



INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

<p>(51) International Patent Classification ⁶ : A61K 31/16, 31/165, 31/415, 31/425, 38/05, C12N 9/48, 9/64, C12Q 1/37</p>	<p>A1</p>	<p>(11) International Publication Number: WO 97/16177</p> <p>(43) International Publication Date: 9 May 1997 (09.05.97)</p>																																																																																						
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(54) Title: **METHOD OF INHIBITING CATHEPSIN K**

Human Cathepsin K

(57) Abstract

A novel cathepsin K crystalline structure is identified. Also disclosed are methods of identifying inhibitors of this protease and methods of inhibiting cathepsin K using inhibitors with certain structural, physical and spatial characteristics.

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METHOD OF INHIBITING CATHEPSIN K

5 Field of the Invention

This invention relates to a method of inhibiting cathepsin K by administering compounds with certain structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of the enzyme. This interaction between the compounds of this invention and the active
10 site inhibits the activity of cathepsin K and these compounds are useful for treating diseases in which said inhibition is indicated, such as osteoporosis and periodontal disease. This invention also relates to a novel crystalline structure of cathepsin K, the identification of a novel protease catalytic active site for this enzyme and methods enabling the design and selection of inhibitors of said active site.

15 Background of the Invention

Cathepsin K is a member of the family of enzymes which are part of the papain superfamily of cysteine proteases. Cathepsins B, H, L, N and S have been described in the literature. Recently, cathepsin K polypeptide and the cDNA
20 encoding such polypeptide were disclosed in U.S. Patent No. 5,501,969 (called cathepsin O therein). Cathepsin K has been recently expressed, purified, and characterized. Bossard, M. J., et al., (1996) *J. Biol. Chem.* **271**, 12517-12524; Drake, F.H., et al., (1996) *J. Biol. Chem.* **271**, 12511-12516; Bromme, D., et al., (1996) *J. Biol. Chem.* **271**, 2126-2132.

25 Cathepsin K has been variously denoted as cathepsin O, cathepsin X or cathepsin O2 in the literature. The designation cathepsin K is considered to be the more appropriate one (name assigned by Nomenclature Committee of the International Union of Biochemistry and Molecular Biology).

Cathepsins of the papain superfamily of cysteine proteases function in the
30 normal physiological process of protein degradation in animals, including humans, e.g., in the degradation of connective tissue. However, elevated levels of these enzymes in the body can result in pathological conditions leading to disease. Thus, cathepsins have been implicated in various disease states, including but not limited to, infections by pneumocystis carinii, trypsanoma cruzi, trypsanoma brucei brucei,
35 and Crithidia fusciculata; as well as in schistosomiasis malaria, tumor metastasis, metachromatic leukodystrophy, muscular dystrophy, amyotrophy, and the like. See International Publication Number WO 94/04172, published on March 3, 1994, and

references cited therein. See also European Patent Application EP 0 603 873 A1, and references cited therein. Two bacterial cysteine proteases from *P. gingivallis*, called gingipains, have been implicated in the pathogenesis of gingivitis. Potempa, J., et al. (1994) *Perspectives in Drug Discovery and Design*, 2, 445-458.

5 Cathepsin K is believed to play a causative role in diseases of excessive bone or cartilage loss. Bone is composed of a protein matrix in which spindle- or plate-shaped crystals of hydroxyapatite are incorporated. Type I Collagen represents the major structural protein of bone comprising approximately 90% of the structural protein. The remaining 10% of matrix is composed of a number of non-collagenous
10 proteins, including osteocalcin, proteoglycans, osteopontin, osteonectin, thrombospondin, fibronectin, and bone sialoprotein. Skeletal bone undergoes remodeling at discrete foci throughout life. These foci, or remodeling units, undergo a cycle consisting of a bone resorption phase followed by a phase of bone replacement.

15 Bone resorption is carried out by osteoclasts, which are multinuclear cells of hematopoietic lineage. The osteoclasts adhere to the bone surface and form a tight sealing zone, followed by extensive membrane ruffling on their apical (i.e., resorbing) surface. This creates an enclosed extracellular compartment on the bone surface that is acidified by proton pumps in the ruffled membrane, and into which
20 the osteoclast secretes proteolytic enzymes. The low pH of the compartment dissolves hydroxyapatite crystals at the bone surface, while the proteolytic enzymes digest the protein matrix. In this way, a resorption lacuna, or pit, is formed. At the end of this phase of the cycle, osteoblasts lay down a new protein matrix that is subsequently mineralized. In several disease states, such as osteoporosis and Paget's
25 disease, the normal balance between bone resorption and formation is disrupted, and there is a net loss of bone at each cycle. Ultimately, this leads to weakening of the bone and may result in increased fracture risk with minimal trauma.

 The abundant selective expression of cathepsin K in osteoclasts strongly suggests that this enzyme is essential for bone resorption. Thus, selective inhibition
30 of cathepsin K may provide an effective treatment for diseases of excessive bone loss, including, but not limited to, osteoporosis, gingival diseases such as gingivitis and periodontitis, Paget's disease, hypercalcemia of malignancy, and metabolic bone disease. Cathepsin K levels have also been demonstrated to be elevated in chondroclasts of osteoarthritic synovium. Thus, selective inhibition of cathepsin K
35 may also be useful for treating diseases of excessive cartilage or matrix degradation.

including, but not limited to, osteoarthritis and rheumatoid arthritis. Metastatic neoplastic cells also typically express high levels of proteolytic enzymes that degrade the surrounding matrix. Thus, selective inhibition of cathepsin K may also be useful for treating certain neoplastic diseases.

5 Surprisingly, it has been found that a broad, structurally diverse series of compounds have common structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of cathepsin K and are useful for treating diseases in which inhibition of bone resorption is indicated, such as osteoporosis and periodontal disease. Thus, this
10 invention relates to the method of inhibiting cathepsin K using compounds having the characteristics hereinbelow defined.

Summary of the Invention

In one aspect, the present invention provides a method for inhibiting
15 cathepsin K by administering compounds with certain structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of the enzyme. This interaction inhibits the activity of cathepsin K and, thus, treats diseases in which bone resorption is a factor.

In another aspect, the present invention provides a novel cysteine protease in
20 crystalline form.

In yet another aspect, the invention provides a novel protease composition characterized by a three dimensional catalytic site formed by the atoms of the amino acid residues listed in Table XXIX.

In still another aspect, the invention provides a method for identifying
25 inhibitors of the compositions described above which methods involve the steps of: providing the coordinates of the protease structure of the invention to a computerized modeling system; identifying compounds which will bind to the structure; and screening the compounds or analogs derived therefrom identified for cathepsin K inhibitory bioactivity.

30 Other aspects and advantages of the present invention are described further in the following detailed description of the preferred embodiments thereof.

Brief Description of the Drawings

Figure 1 is the amino acid sequence of cathepsin K aligned with the amino
35 acid sequences of other cysteine proteases.

Figure 2 is a ribbon diagram of cathepsin K. The amino and carboxyl-termini are indicated by N and C. The drawing was produced using the program MOLSCRIPT [Kraulis, P., *J. Appl. Crystallogr.*, 24, 946-950 (1991)].

Figure 3 is a ribbon diagram of cathepsin K in complex with E-64, a known inhibitor of cysteine proteases. The drawing was produced using the program MOLSCRIPT.

Figure 4a is an illustration of the active site of cathepsin K. Figure 4b is a stereoview of the active site of cathepsin K. For clarity, no hydrogen atoms or water molecules are shown.

Figures 5a-13a are illustrations of the active site of cathepsin K in complex with novel inhibitors of cathepsin K. Figures 5b-13b are stereoviews of the active site of cathepsin K in complex with novel inhibitors of cathepsin K. These views depict the interaction of each inhibitor with all atoms of residues of the active site of cathepsin K within 5 Å of the inhibitors. For clarity, no hydrogen atoms or water molecules are shown.

Table I provides the three dimensional protein coordinates of the cathepsin K crystalline structure of the invention.

Tables II-X provide the three dimensional coordinates for the cathepsin K complex with specific inhibitors of the present invention.

Tables XI-XIX provide listings of the three atom angles between atoms of the inhibitors and the protein for all inhibitor atoms within 5 Ångstroms of the protein.

Tables XX-XXVIII provide listings of the distances between atoms of the inhibitors and the protein for all inhibitor atoms within 5 Ångstroms of the protein.

Table XXIX provides the atoms of the amino acid residues of the catalytic site.

Detailed Description of the Invention

The present invention provides a novel cysteine protease crystalline structure, a novel cysteine protease active site, and methods of use of the crystalline form and active site to identify protease inhibitor compounds.

In particular, the present invention provides a method for inhibiting cathepsin K by administering compounds with certain structural, physical and spatial characteristics that allow for the interaction of said compounds with specific residues

Specifically, the inhibitors of cathepsin K used in the present invention interact with any two or more of the following:

1. Tyrosine 67 sidechain;
2. Hydrophobic pocket lined with atoms from methionine 68,
5 leucine 209, alanine 163, alanine 134 and portions of tyrosine 67;
3. Hydrogen bonds donated by glycine 66 amide nitrogen;
4. Cysteine 25 the active site nucleophile;
5. Mainchain interactions from residues glutamine 21, cysteine 22, and
glycine 23;
- 10 6. Tryptophan 184 sidechain; and
7. Hydrophobic contacts with the sidechain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138.

Preferably, the inhibitors of cathepsin K used in the present invention interact with any three or more of the above-identified regions of the active site.

- 15 The compounds used in the methods of the present invention possess an electrophilic carbon and either a hydrophobic group whose centroid is 5.44-6.94Å from the carbon or an aromatic group whose centroid is 9.24-11.24Å from the carbon, or both the hydrophobic and the aromatic groups in which case the centroids of these two groups should be 15.67-16.67Å apart. These features must be able to
20 make the appropriate interactions with the cathepsin K active site. The electrophilic carbon atom should be 1.7-4.0Å from the side chain sulfur atom (SG) on the amino acid cysteine 25. The hydrophobic group should be near the following amino acids with appropriate distance ranges between the centroid of the side chain atoms and the centroid of the hydrophobic group given in parentheses: tyrosine 67 (4.91-
25 5.91Å), methionine 68 (5.74-6.74Å), alanine 134 (4.15-5.15Å), leucine 160 (6.18-7.18Å), and leucine 209 (5.71-6.71Å). The aromatic group should be near the either tryptophan 184 (4.10-7.10Å) or tryptophan 188 (4.10-7.10Å) or both.

- The key structural features of the inhibitors of the present invention include an electrophilic carbon, preferably the carbon of a carbonyl group, a hydrophobic
30 group, preferably an isobutyl group, and an aromatic group, preferably a phenyl group. The electrophilic carbon of the inhibitor may be in the same compound with two hydrophobic groups, such as two isobutyl groups, or two aromatic groups, such as two phenyl groups, or one hydrophobic group and one aromatic group.

- Suitably, the method of inhibiting cathepsin K of the present invention
35 comprises administering to a mammal, preferably a human, in need thereof a

compound that fits spatially into the active site of cathepsin K, said compound comprising any two or more of the following:

- 5 (i) an electrophilic carbon atom that binds to the side chain sulfur atom of cysteine 25 wherein said electrophilic carbon atom is 1.7-4.0Å from said sulfur atom;
- (ii) a hydrophobic group that interacts with tryptophan 184 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tryptophan 184 is 4.10-7.10Å;
- 10 (iii) a hydrophobic group that interacts with tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209, creating a hydrophobic pocket, and has distance ranges between the centroid of said hydrophobic group and the centroids of the side chain atoms of the amino acid residues of said hydrophobic pocket which are tyrosine 67: 4.91- 5.91Å, methionine 68: 5.74-6.74Å, alanine 134: 4.15-5.15Å, leucine 160: 6.18-7.18Å, and leucine 209: 5.71-6.71Å;
- 15 (iv) a hydrophobic group that interacts with tyrosine 67 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tyrosine 67 is 4.10-7.10Å;
- (v) an amino group with a pKa of less than 7 or an oxygen atom, each of which interacts with a hydrogen atom donated by the amide nitrogen of glycine 66
20 wherein the distance between these two atoms is 2.7-3.5Å;
- (vi) a hydrophobic group that interacts with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 wherein the distance between the centroid of said hydrophobic group and the centroids of glutamine 21, cysteine 22 and glycine 23 are 3.7-5.4, 4.9-5.7 and 5.4-6.7Å, respectively; or
- 25 (vii) a hydrophobic group that interacts with the side chain atoms of glutamine 143 and asparagine 161 and the main chain of alanine 137 and serine 138 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 143, asparagine 161, alanine 137, and serine 138 are 7.9-9.6Å, 4.7-5.4Å, 4.2-5.5Å, and 4.6-6.4Å, respectively. Preferably, the inhibitors of
30 cathepsin K used in the present invention comprise three or more of the above.

Suitably, the method of inhibiting cathepsin K of the present invention comprises administering to a mammal, preferably a human, in need thereof, a compound that fits spatially into the active site of cathepsin K, said compound comprising:

(i) an electrophilic carbon atom that binds to the side chain sulfur atom of cysteine 25 wherein said electrophilic carbon atom is 1.7-4.0Å from said sulfur atom; and

(ii) a hydrophobic group that interacts with tryptophan 184 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tryptophan 184 is 4.10-7.10Å. Preferably, the hydrophobic group that interacts with tryptophan 184 is an aromatic group and the centroid of this aromatic group is 9.24-11.24Å from the centroid of the electrophilic carbon that binds to the side chain sulfur atom of cysteine 25.

Preferably, the electrophilic carbon that binds to the side chain sulfur atom of cysteine 25 is a carbonyl carbon.

Suitably, the method of the present invention further comprises a compound with a hydrophobic group that:

has a centroid which is 5.44-6.94Å from said electrophilic carbon;
interacts with tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209, creating a hydrophobic pocket; and

has distance ranges between the centroid of said hydrophobic group and the centroids of the side chain atoms of the amino acid residues of said hydrophobic pocket which are tyrosine 67: 4.91- 5.91Å, methionine 68: 5.74-6.74Å, alanine 134: 4.15-5.15Å, leucine 160: 6.18-7.18Å, and leucine 209: 5.71-6.71Å. Preferably, this hydrophobic group is an isobutyl group.

Alternately, the method of the present invention further comprises a compound with a hydrophobic group that interacts with tyrosine 67 wherein the distance between the centroid of said hydrophobic group and the centroid of the side chain atoms of tyrosine 67 is 4.10-7.10Å. Preferably, this hydrophobic group is an aromatic group.

Alternately, the method of the present invention further comprises a compound with an amino group with a pKa of less than 7 or an oxygen atom, each of which interacts with a hydrogen atom donated by the amide nitrogen of glycine 66 wherein the distance between these two atoms is 2.7-3.5Å. Preferably, the compound comprises an oxygen atom, such as an oxygen atom of a carbonyl group or an oxygen atom of a hydroxyl group.

Alternately, the method of the present invention further comprises a compound with a hydrophobic group that interacts with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 wherein the distance between the centroid

of the hydrophobic group and the centroids of glutamine 21, cysteine 22 and glycine 23 are 3.7-5.4, 4.9-5.7 and 5.4-6.7 Å, respectively. Preferably, this hydrophobic group is an isobutyl group.

Alternately, the method of the present invention further comprises a compound with a hydrophobic group that interacts with the side chain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138 wherein the distance between the centroid of the hydrophobic group and the centroids of glutamine 143, asparagine 161, alanine 137, and serine 138 are 7.9-9.6 Å, 4.7-5.4 Å, 4.2-5.5 Å, and 4.6-6.4 Å, respectively.

Compounds used in the method of the present invention include, but are not limited to, the following:

3(S)-3-[(N-benzyloxycarbonyl)-L-leuciny]amino-5-methyl-1-(1-propoxy)-2-hexanone;

4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone;

4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N-[N-(methyl)-L-leucyl]-3-pyrrolidinone;

4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone;

bis-(Cbz-leuciny)-1,3-diamino-propan-2-one;

2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl)-L-leuciny]]carbohydrazide;

(1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leuciny)]hydrazide;

1-N-(N-imidazole acetyl-leuciny)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one; and

2,2'-N,N'-bis-benzyloxycarbonyl-L-leuciny]carbohydrazide;

or a pharmaceutically acceptable salt thereof.

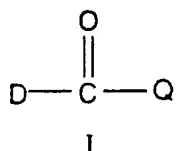
As stated herein, the interaction of the inhibitor at the side chain sulfur atom of cysteine 25 has as one of its requirements that the inhibitor contain an "electrophilic carbon" atom. By this term is meant an electron deficient carbon. This term includes, but is not limited to, a carbonyl carbon atom. This term also includes an epoxide, a thiocarbonyl, an imine, and a nitrile. Suitably, this term may also be represented by the formula $-C=N-X$, wherein X may be optionally tied back to C in a ring or wherein X is CH_2 , H, O, S or NR^a in which R^a is H or C_{1-4} alkyl.

includes an epoxide, a thiocarbonyl, an imine, and a nitrile. Suitably, this term may also be represented by the formula $-C=N-X$, wherein X may be optionally tied back to C in a ring or wherein X is CH_2 , H, O, S or NR^a in which R^a is H or C_{1-4} alkyl.

The hydrophobic groups that interact with tryptophan 184 or tyrosine 67 include, but are not limited to, aromatic groups. These hydrophobic groups include phenyl, C_{1-6} alkyl and heteroaryl, which is defined hereinbelow. The hydrophobic groups that interact with the hydrophobic pocket lined with atoms from tyrosine 67, methionine 68, alanine 134, leucine 160, and leucine 209 not only includes isobutyl, but also includes C_{1-6} alkyl, C_{3-6} cycloalkyl and adamantyl. The hydrophobic groups that interact with the main chain atoms of glutamine 21, cysteine 22 and glycine 23 or the side chain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138 include C_{1-10} alkyl, C_bF_{2b+1} , in which b is 1-3, and aryl and heteroaryl, each of which are defined hereinbelow.

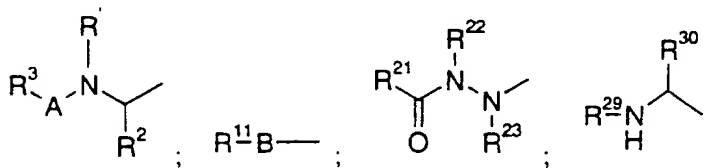
As used herein, the term "centroid" means the position for the stated atoms calculated by averaging the x coordinates of the atoms to obtain the x coordinate of the centroid, averaging the y coordinates of the atoms to obtain the y coordinate of the centroid, and averaging the z coordinates of the atoms to obtain the z coordinate of the centroid.

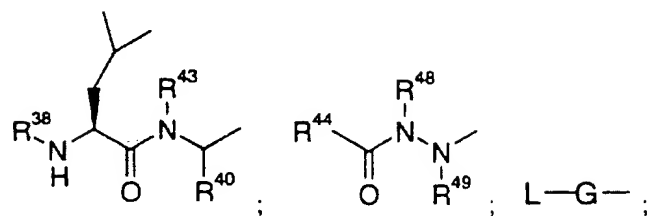
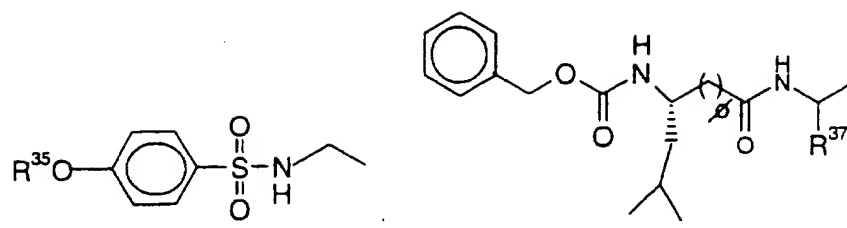
The compounds used in the method of the present invention include, but are not limited to, the compounds of formula (I):



wherein:

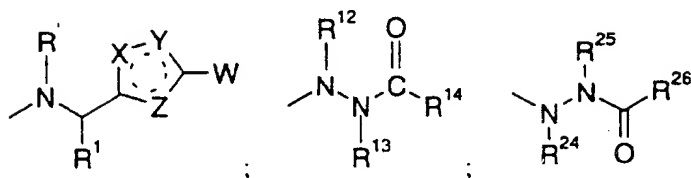
25 D =



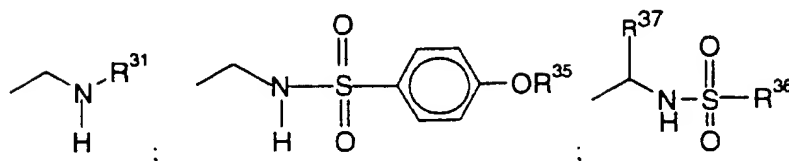


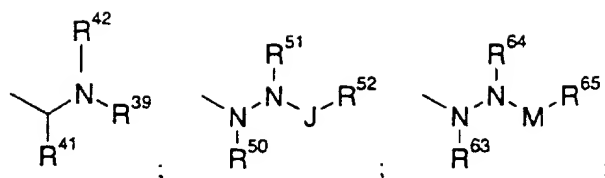
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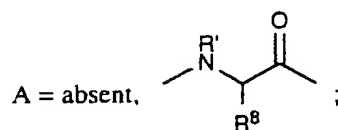


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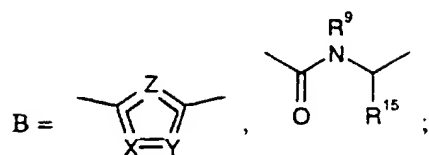




where:



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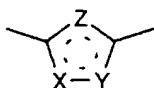


L = C₂₋₆alkyl, Ar-C₀₋₆alkyl, Het-C₀₋₆alkyl, CH(R⁶⁶)NR⁶⁰R⁶⁸,
CH(R⁶⁶)Ar, CH(R⁶⁶)OAr, NR⁶⁶R⁶⁷;

10

M = C(O), SO₂;

G =



J = C(O), SO₂;

15

T = Ar, Het;

V = C₃₋₇cycloalkyl;

W = H, -CN, -CF₃, -NO₂, -COR⁷, -CO₂R⁶, -CONHR⁶,
-SO₂NHR⁶, -NHCO₂R⁶, -NHCOR⁷, -O-COR⁶, -SR⁶,
NR'R⁶, NR'(C=NH)NHR⁵, Cl, Br, I, F;

$X = Y = Z = N, O, S$ or CR^4 ,

provided that at least two of X, Y and Z are heteroatoms
and at least one of X, Y and Z is N, or one of X, Y and Z is
 $C=N$, $C=C$ or $N=N$ and the other two are CR^4 or N,

5 provided that X, Y and Z together comprise at least two N;

\equiv indicates a single or double bond in the five-membered
heterocycle;

$m = 0, 1, 2$;

$n = 1$ to 6;

10 $f = 0, 1, 2$;

Ar = phenyl, naphthyl, optionally substituted by one or more of
Ph- C_{0-6} alkyl, Het- C_{0-6} alkyl, C_{1-6} alkoxy, Ph- C_{0-6} alkoxy,
Het- C_{0-6} alkoxy, OH, $(CH_2)_{1-6}NR^{58}R^{59}$,
 $O(CH_2)_{1-6}NR^{58}R^{59}$;

15 Ar' = phenyl or naphthyl, optionally substituted by one or more of
Ph- C_{0-6} alkyl, Het- C_{0-6} alkyl, C_{1-6} alkoxy, Ph- C_{0-6} alkoxy,
Het- C_{0-6} alkoxy, OH, $(CH_2)_{1-6}NR^{58}R^{59}$,
 $O(CH_2)_{1-6}NR^{58}R^{59}$, or halogen;

R' = H, C_{1-6} alkyl, Ar- C_{0-6} alkyl, Het- C_{0-6} alkyl;

20 $R^1 = H, C_{1-6}$ alkyl;

$R^2 = C_{4-6}$ alkyl, C_{4-6} alkenyl, benzyl;

$R^3 = C_{1-6}$ alkyl, Ar- C_{0-6} alkyl, Het- C_{0-6} alkyl, R^5CO- , R^5SO_2- ,
 $R^5OC(O)-$, R^5NHCO- ;

$R^4 = H, C_{1-6}$ alkyl, Ar- C_{0-6} alkyl, Het- C_{0-6} alkyl;

25 $R^5 = Ar-O-6$ alkyl, Het- C_{0-6} alkyl;

$R^6 = H, C_{1-6}$ alkyl, CH_2CF_3 , Ar- C_{0-6} alkyl, Het- C_{0-6} alkyl;

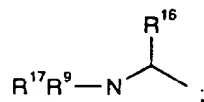
$R^7 = C_{1-6}\text{alkyl}, \text{Ar-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl};$

$R^8 = \text{H}; C_{2-6}\text{alkenyl}; C_{2-6}\text{alkynyl}; \text{Het}; \text{Ar}; C_{1-6}\text{alkyl},$
 optionally substituted by $\text{OR}', \text{SR}', \text{NR}'_2, \text{CO}_2\text{R}',$
 $\text{CO}_2\text{NR}'_2, \text{N}(\text{C}=\text{NH})\text{NH}_2, \text{Het}$ or $\text{Ar};$

5 $R^9 = \text{H}, C_{1-6}\text{alkyl}, \text{Ar-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl};$

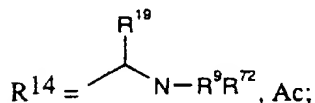
$R^{10} = C_{1-6}\text{alkyl}, \text{Ar-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl};$

$R^{11} = \text{H}, C_{1-6}\text{alkyl}, \text{Ar-C}_{1-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl},$ or



$R^{12} = \text{H}, C_{1-6}\text{alkyl}, \text{Ar-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl};$

10 $R^{13} = \text{H}, C_{1-6}\text{alkyl}, \text{Ar-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl};$



$R^{15} = \text{H}, C_{1-6}\text{alkyl}, C_{2-6}\text{alkenyl}, C_{2-6}\text{alkynyl}, \text{Ar}, \text{Het},$ or

$C_{1-6}\text{alkyl}$ optionally substituted by $\text{OR}^9, \text{NR}^9_2,$

$\text{CONR}^9_2, \text{N}(\text{C}=\text{NH})\text{NH}-, \text{Het}$ or $\text{Ar};$

15 $R^{16} = C_{2-6}\text{alkyl}, C_{2-6}\text{alkenyl}, C_{2-6}\text{alkynyl}, \text{Ar}, \text{Het},$ or $C_{2-6}\text{alkyl}$

optionally substituted by $\text{OR}^9, \text{SR}^9, \text{NR}^9_2, \text{CO}_2\text{R}^9,$

$\text{CONR}^9_2, \text{N}(\text{C}=\text{NH})\text{NH}-, \text{Het}$ or $\text{Ar};$

$R^{19} = \text{H}, C_{1-6}\text{alkyl}, C_{2-6}\text{alkenyl}, C_{2-6}\text{alkynyl}, \text{Ar}, \text{Het},$ or $C_{1-6}\text{alkyl}$

optionally substituted by $\text{OR}^9, \text{SR}^9, \text{NR}^9_2, \text{CO}_2\text{R}^9, \text{CONR}^9_2,$

20 $\text{N}(\text{C}=\text{NH})\text{NH}-, \text{Het}$ or $\text{Ar};$

$R^{17} = R^{72} = \text{H}, C_{1-6}\text{alkyl}, R^{10}, R^{10}\text{C}(\text{O})-, R^{10}\text{C}(\text{S})-, R^{10}\text{OC}(\text{O})-;$

$R^{21} = R^{26} = C_{5-6}\text{alkyl}; C_{2-6}\text{alkenyl}; C_{3-11}\text{cycloalkyl}; T\text{-}C_{3-6}\text{alkyl}; V\text{-}C_{1-6}\text{alkyl}; T\text{-}C_{2-6}\text{alkenyl};$
 $T\text{-}(CH_2)_nCH(T)(CH_2)_n$; optionally substituted by one or two halogens, SR^{20} , OR^{20} , $NR^{20}R^{27}$ or $C_{1-4}\text{alkyl}$;

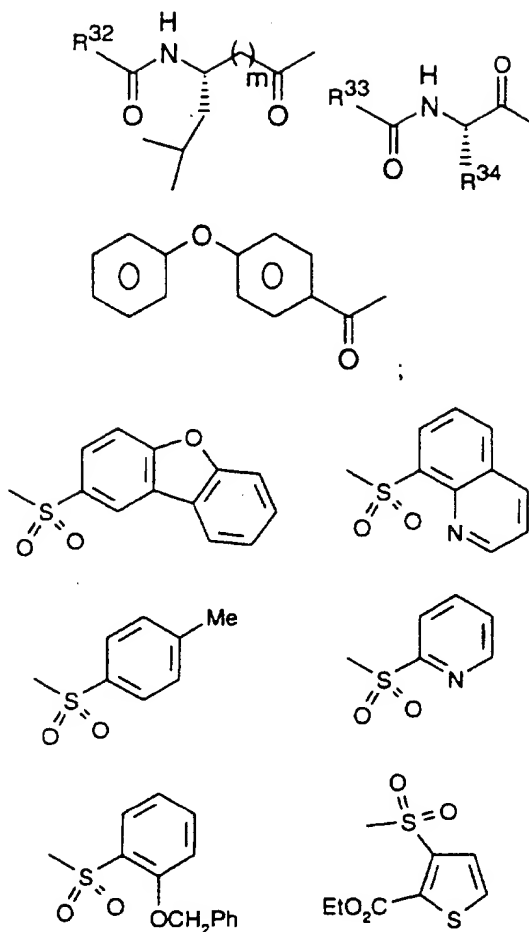
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$R^{27} = R^{28}CO, R^{28}OCO$;

$R^{28} = C_{1-6}\text{alkyl}; C_{3-11}\text{cycloalkyl}; Ar; Het; T\text{-}C_{1-6}\text{alkyl};$
 $T\text{-}(CH_2)_nCH(T)(CH_2)_n$; optionally substituted by one or two halogens, SR^{20} , OR^{20} , $NR^{20}R^{73}$, $C_{1-6}\text{alkyl}$;

10

$R^{20} = R^{22} = R^{23} = R^{24} = R^{25} = R^{73} = H, C_{1-4}\text{alkyl}, Ar\text{-}C_{0-6}\text{alkyl},$
 $Het\text{-}C_{0-6}\text{alkyl};$

R²⁹ =

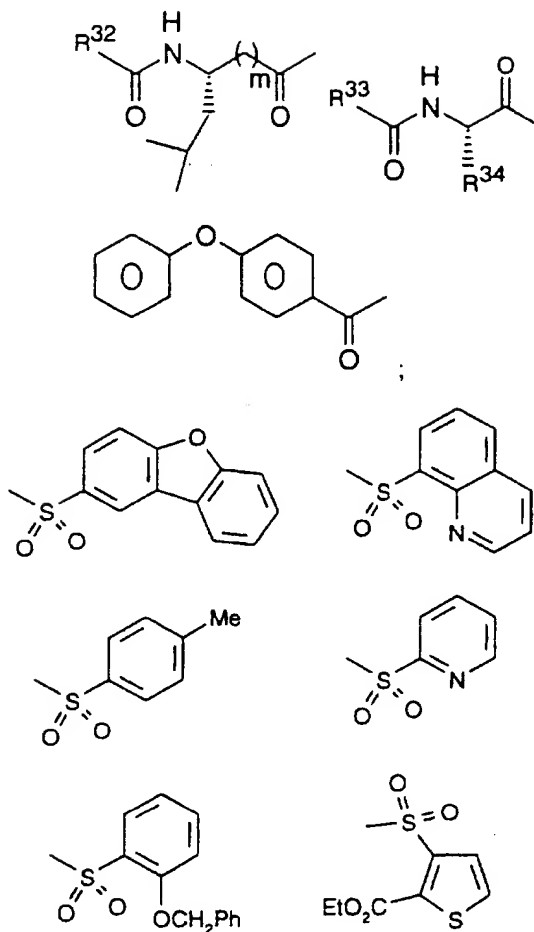
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10

Cbz-leuciny-; 2-, 3-, or 4-pyridyl methyloxycarbonyl-leuciny-; 4-imidazole
 acetyl-leuciny-, phenyl acetyl-leuciny-, N,N-dimethyl-glyciny- leuciny-, 4-
 pyridyl acetyl-leuciny-, 2-pyridyl sulfonyl-leuciny-, 4-pyridyl carbonyl-
 leuciny-, acetyl-leuciny-, benzoyl-leuciny-, 4-phenoxy-benzoyl-, 2- or 3-
 benzyloxybenzoyl-, biphenyl acetyl-, lpha- isobutyl-biphenyl acetyl-, Cbz-
 phenylalaniny-, Cbz-norleuciny-, Cbz-norvaliny-, Cbz-glutaminy-, Cbz-

epsilon- (t-butyl ester)-glutamyl; acetyl-leucinyl-, 6- or 8- quinoline
carbonyl, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, acetyl, benzoyl, 2-
or 3- benzyloxy benzoyl, 4-phenoxy benzoyl-, Cbz-amino acid-; 2-,3-, or 4-
pyridylmethyloxycarbonyl-aminoacid-; aryl C₀-C₆alkyloxy carbonyl-amino
5 acid-, heteroaryl C₀-C₆alkyloxy carbonyl-amino acid-, aryl C₀-C₆alkyloxy
carbonyl-amino acid-, heteroaryl C₀-C₆alkyloxy carbonyl-amino acid-, C₁-
C₆alkyloxy carbonyl-amino acid-; C₁-C₆alkyl carbonyl, aryl C₀-C₆alkyl
carbonyl, heteroaryl C₀-C₆alkyl carbonyl, aryl C₀-C₆alkyl carbonyl,
heteroaryl C₀-C₆alkyl carbonyl, C₁-C₆alkyl sulfonyl, aryl C₀-C₆alkyl
10 sulfonyl, heteroaryl C₀-C₆alkyl sulfonyl, aryl C₀-C₆alkyl sulfonyl,
heteroaryl C₀-C₆alkyl sulfonyl;

R³⁰ = -H, C₁₋₆ alkyl;

R³¹ =

5

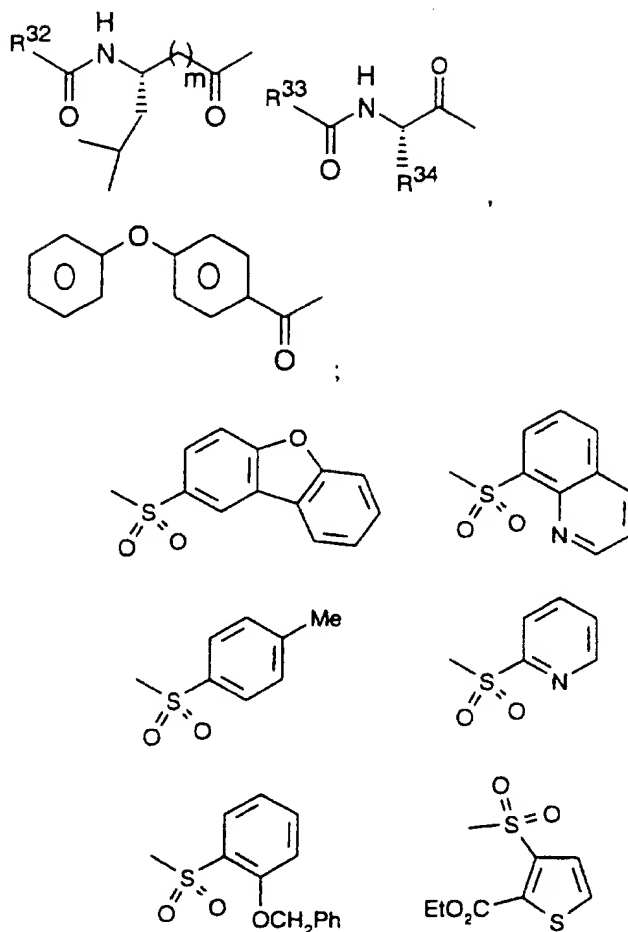
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Cbz-leuciny-; 2-, 3-, or 4-pyridyl methoxycarbonyl-leuciny-; 4-imidazole acetyl-leuciny-, phenyl acetyl-leuciny-, N,N-dimethyl-glyciny- leuciny-, 4-pyridyl acetyl-leuciny-, 2-pyridyl sulfonyl-leuciny-, 4-pyridyl carbonyl-leuciny-, acetyl-leuciny-, benzoyl-leuciny-, 4-phenoxy-benzoyl-, 2- or 3-benzyloxybenzoyl-, biphenyl acetyl-, alpha- isobutyl-biphenyl acetyl-, Cbz-phenylalaniny-, Cbz-norleuciny-, Cbz-norvaliny-, Cbz-glutaminy-, Cbz-

epsilon- (t-butyl ester)-glutamyl; acetyl-leuciny-, 6- or 8- quinoline
 carbonyl, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, acetyl, benzoyl, 2-
 or 3- benzyloxy benzoyl, 4-phenoxy benzoyl-, Cbz-amino acid-; 2-,3-, or 4-
 pyridylmethyloxycarbonyl-aminoacid-; aryl C₀-C₆alkyloxy carbonyl-amino
 5 acid-, heteroaryl C₀-C₆alkyloxy carbonyl-amino acid-, aryl C₀-C₆alkyloxy
 carbonyl-amino acid-, heteroaryl C₀-C₆alkyloxy carbonyl-amino acid-,
 C₁-C₆alkyloxy carbonyl-amino acid-; C₁-C₆alkyl carbonyl, aryl C₀-C₆alkyl
 carbonyl, heteroaryl C₀-C₆alkyl carbonyl, aryl C₀-C₆alkyl carbonyl,
 heteroaryl C₀-C₆alkyl carbonyl, C₁-C₆alkyl sulfonyl, aryl C₀-C₆alkyl
 10 sulfonyl, heteroaryl C₀-C₆alkyl sulfonyl, aryl C₀-C₆alkyl sulfonyl,
 heteroaryl C₀-C₆alkyl sulfonyl;

R³² = OCH₂Ar, OCH₂C₁₋₆alkyl, aryl substituted C₀₋₆alkyl,
 heteroaryl substituted C₀₋₆alkyl, 4-imidazole methylene; 2-,
 3-, or 4-pyridylmethylenedioxy; 4-pyridyl methylene, 2-
 15 pyridyl sulfonyl, 4-pyridyl, aryl substituted C₀₋₆alkyloxy,
 heteroaryl substituted C₀₋₆alkyloxy;

R³³ = C₁₋₆alkyl, -CH₂Ph, -CH₂CH₂CO₂R³⁴;
 R³⁴ = -H, C₁₋₆alkyl;
 R³⁵ = Ar, HetAr;
 20 R³⁶ = Aryl, heteroaryl, pyridyl, isoquinolinyl;
 R³⁷ = C₁₋₆alkyl, -CH₂Ph, -CH₂CH₂CO₂R³⁴;
 R³⁸ = Cbz; C₁₋₆alkyl or aryl substituted
 Cbz; C₁₋₆alkyl -CO; benzoyl; C₁₋₆alkyl or aryl
 substituted benzoyl;

$R^{39} =$


5

Cbz-leuciny-; 2-, 3-, or 4-pyridyl methyloxycarbonyl-leuciny-; 4-imidazole
 acetyl-leuciny-, phenyl acetyl-leuciny-, N,N-dimethyl-glyciny- leuciny-, 4-
 pyridyl acetyl-leuciny-, 2-pyridyl sulfonyl-leuciny-, 4-pyridyl carbonyl-
 leuciny-, acetyl-leuciny-, benzoyl-leuciny-, 4-phenoxy-benzoyl-, 2- or 3-
 benzyloxybenzoyl-, biphenyl acetyl-, alpha- isobutyl-biphenyl acetyl-, Cbz-
 phenylalaniny-, Cbz-norleuciny-, Cbz-norvaliny-, Cbz-glutaminy-, Cbz-

10

epsilon- (t-butyl ester)-glutamyl; acetyl-leuciny-, 6- or 8- quinoline
 carbonyl, biphenyl acetyl, alpha- isobutyl-biphenyl acetyl, acetyl, benzoyl, 2-
 or 3- benzyloxy benzoyl, 4-phenoxy benzoyl-, Cbz-amino acid-; 2-,3-, or 4-
 pyridylmethyloxycarbonyl-aminoacid-; aryl C₀-C₆alkyloxy carbonyl-amino
 5 acid-, heteroaryl C₀-C₆alkyloxy carbonyl-amino acid-, aryl C₀-C₆alkyloxy
 carbonyl-amino acid-, heteroaryl C₀-C₆alkyloxy carbonyl-amino acid-, C₁-
 C₆alkyloxy carbonyl-amino acid-; C₁-C₆alkyl carbonyl, aryl C₀-C₆alkyl
 carbonyl, heteroaryl C₀-C₆alkyl carbonyl, aryl C₀-C₆alkyl carbonyl,
 heteroaryl C₀-C₆alkyl carbonyl, C₁-C₆alkyl sulfonyl, aryl C₀-C₆alkyl
 10 sulfonyl, heteroaryl C₀-C₆alkyl sulfonyl, aryl C₀-C₆alkyl sulfonyl,
 heteroaryl C₀-C₆alkyl sulfonyl;

R⁴⁰ = H and C₁-6alkyl;

R⁴¹ = H and C₁-6alkyl;

R⁴² = C₁-6alkyl, aryl substituted C₁-6alkyl and hetero aryl
 15 substituted C₁-6alkyl,; H when R⁴³ is C₁-6alkyl, aryl substituted
 C₁-6alkyl; and heteroaryl substituted C₁-6alkyl;

R⁴³ = C₁-6alkyl, aryl substituted C₁-6alkyl and hetero aryl
 substituted C₁-6alkyl,; H when R⁴² is C₁-6alkyl, aryl substituted
 C₁-6alkyl; and heteroaryl substituted C₁-6alkyl;

R⁴⁴ = CH(R⁵³)NR⁴⁵R⁵⁴, CH(R⁵⁵)Ar, C₅-6alkyl;

R⁴⁵ = R⁴⁶ = R⁴⁷ = R⁴⁸ = R⁴⁹ = R⁵⁰ = R⁵¹ = H, C₁-6alkyl,

Ar-C₀-6alkyl, Het-C₀-6alkyl;

R⁵² = Ar, Het, CH(R⁵⁶)Ar, CH(R⁵⁶)OAr, N(R⁵⁶)Ar, C₁-6alkyl,

CH(R⁵⁶)NR⁴⁶R⁵⁷;

$R^{53} = C_{2-6}\text{alkyl}, \text{Ar-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl},$

R^{53} and R^{45} may be connected to form a pyrrolidine or piperidine ring;

$R^{54} = R^{57} = R^{47}, R^{47}C(O), R^{47}C(S), R^{47}OC(O);$

5 $R^{55} = R^{56} = R^{58} = R^{59} = H, C_{1-6}\text{alkyl}, \text{Ar-C}_{0-6}\text{alkyl},$
 $\text{Het-C}_{0-6}\text{alkyl};$

$R^{60} = R^{61} = R^{62} = R^{63} = R^{64} = H, C_{1-6}\text{alkyl},$

$\text{Ar-C}_{0-6}\text{alkyl}, \text{or Het-C}_{0-6}\text{alkyl};$

$R^{65} = C_{1-6}\text{alkyl}, \text{Ar}, \text{Het}, \text{CH}(R^{69})\text{Ar}, \text{CH}(R^{69})\text{OAr}, \text{N}(R^{69})\text{Ar},$

10 $\text{CH}(R^{69})\text{NR}^{61}\text{R}^{70};$

$R^{66} = R^{69} = R^{71} = H, C_{1-6}\text{alkyl}, (\text{CH}_2)_{0-6}\text{-C}_{3-6}\text{cycloalkyl},$

$\text{Ar-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl};$

$R^{67} = C_{1-6}\text{alkyl}, (\text{CH}_2)_{0-6}\text{-C}_{3-6}\text{cycloalkyl}, \text{Ar-C}_{0-6}\text{alkyl},$

15 $\text{Het-C}_{0-6}\text{alkyl}; R^{66}$ and R^{67} may be combined to form
 a 3-7 membered monocyclic or 7-10-membered bicyclic
 carbocyclic or heterocyclic ring, optionally substituted with
 1-4 of $C_{1-6}\text{alkyl}, \text{Ph-C}_{0-6}\text{alkyl}, \text{Het-C}_{0-6}\text{alkyl}, C_{1-6}\text{alkoxy},$
 $\text{Ph-C}_{0-6}\text{alkoxy}, \text{Het-C}_{0-6}\text{alkoxy}, \text{OH}, (\text{CH}_2)_{1-6}\text{NR}^{58}\text{R}^{59},$
 $\text{O}(\text{CH}_2)_{1-6}\text{NR}^{58}\text{R}^{59};$

20 $R^{68} = R^{70} = R^{62}, R^{62}C(O), R^{62}C(S), R^{62}OC(O),$

$R^{62}OC(O)\text{NR}^{59}\text{CH}(R^{71})(\text{CO});$

and pharmaceutically acceptable salts thereof.

25 The compounds of Formula I are hydrazidyl, bis-hydrazidyl and bis-aminomethyl carbonyl compounds having in common key structural features required of protease substrates, most particularly cathepsin K substrates. These structural features endow the present compounds with the appropriate molecular shape necessary to fit into the enzymatic active site, to bind to such active site,

thereby blocking the site and inhibiting enzymatic biological activity. Referring to Formula I, such structural features include the central electrophilic carbonyl, a peptidyl or peptidomimetic molecular backbone on either side of the central carbonyl, a terminal carbobenzyloxy moiety (e.g., Cbz-leuciny), or a mimic thereof, on the backbone on one or both sides of the carbonyl, and optionally, an isobutyl side chain extending from the backbone on one or both sides of the carbonyl.

Abbreviations and symbols commonly used in the peptide and chemical arts are used herein to describe the compounds of the present invention. In general, the amino acid abbreviations follow the IUPAC-IUB Joint Commission on Biochemical Nomenclature as described in *Eur. J. Biochem.*, 158, 9 (1984). The term "amino acid" as used herein refers to the D- or L- isomers of alanine, arginine, asparagine, aspartic acid, cysteine, glutamine, glutamic acid, glycine, histidine, isoleucine, leucine, lysine, methionine, phenylalanine, proline, serine, threonine, tryptophan, tyrosine and valine.

"C₁₋₆alkyl" as applied herein is meant to include substituted and unsubstituted methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl and t-butyl, pentyl, n-pentyl, isopentyl, neopentyl and hexyl and the simple aliphatic isomers thereof. Any C₁₋₆alkyl group may be optionally substituted independently by one or two halogens, SR', OR', N(R')₂, C(O)N(R')₂, carbamyl or C₁₋₄alkyl, where R' is C₁₋₆alkyl. C₀alkyl means that no alkyl group is present in the moiety. Thus, Ar-C₀alkyl is equivalent to Ar.

"C₃₋₁₁cycloalkyl" as applied herein is meant to include substituted and unsubstituted cyclopropane, cyclobutane, cyclopentane, cyclohexane, cycloheptane, cyclooctane, cyclononane, cyclodecane, cycloundecane.

"C₂₋₆alkenyl" as applied herein means an alkyl group of 2 to 6 carbons wherein a carbon-carbon single bond is replaced by a carbon-carbon double bond. C₂₋₆alkenyl includes ethylene, 1-propene, 2-propene, 1-butene, 2-butene, isobutene and the several isomeric pentenes and hexenes. Both cis and trans isomers are included.

"C₂₋₆alkynyl" means an alkyl group of 2 to 6 carbons wherein one carbon-carbon single bond is replaced by a carbon-carbon triple bond. C₂₋₆alkynyl includes acetylene, 1-propyne, 2-propyne, 1-butyne, 2-butyne, 3-butyne and the simple isomers of pentyne and hexyne.


"Halogen" means F, Cl, Br, and I.

"Ar" or "aryl" means phenyl or naphthyl, optionally substituted by one or more of Ph-C₀₋₆alkyl, Het-C₀₋₆alkyl, C₁₋₆alkoxy, Ph-C₀₋₆alkoxy, Het-C₀₋₆alkoxy, OH, (CH₂)₁₋₆NR⁵⁸R⁵⁹, O(CH₂)₁₋₆NR⁵⁸R⁵⁹; where R⁵⁸, R⁵⁹ is H, C₁₋₆alkyl, Ar-C₀₋₆alkyl; Het-C₀₋₆alkyl, from C₁₋₄alkyl, OR', N(R')₂, SR', CF₃, NO₂, CN, CO₂R', CON(R'), F, Cl, Br and I.

As used herein "Het" or "heterocyclic" represents a stable 5- to 7-membered monocyclic or a stable 7- to 10-membered bicyclic heterocyclic ring, which is either saturated or unsaturated, and which consists of carbon atoms and from one to three heteroatoms selected from the group consisting of N, O and S, and wherein the nitrogen and sulfur heteroatoms may optionally be oxidized, and the nitrogen heteroatom may optionally be quaternized, and including any bicyclic group in which any of the above-defined heterocyclic rings is fused to a benzene ring. The heterocyclic ring may be attached at any heteroatom or carbon atom which results in the creation of a stable structure, and may optionally be substituted with one or two moieties selected from C₁₋₄alkyl, OR', N(R')₂, SR', CF₃, NO₂, CN, CO₂R', CON(R'), F, Cl, Br and I, where R' is C₁₋₆alkyl. Examples of such heterocycles include piperidinyl, piperazinyl, 2-oxopiperazinyl, 2-oxopiperidinyl, 2-oxopyrrolidinyl, 2-oxoazepinyl, azepinyl, pyrrolyl, 4-piperidonyl, pyrrolidinyl, pyrazolyl, pyrazolidinyl, imidazolyl, pyridyl, pyrazinyl, oxazolidinyl, oxazolinyl, oxazolyl, isoxazolyl, morpholinyl, thiazolidinyl, thiazolinyl, thiazolyl, quinuclidinyl, indolyl, quinolinyl, isoquinolinyl, benzimidazolyl, benzopyranyl, benzoxazolyl, furyl, pyranyl, tetrahydrofuryl, tetrahydropyranyl, thienyl, benzoxazolyl, thiamorpholinyl sulfoxide, thiamorpholinyl sulfone, and oxadiazolyl.

"HetAr" or "heteroaryl" means any heterocyclic moiety encompassed by the above definition of Het which is aromatic in character, e.g., pyridine.



It will be appreciated that the heterocyclic ring, , includes thiazoles, oxazoles, triazoles, thiadiazoles, oxadiazoles, isoxazoles, isothiazols, imidazoles, pyrazines, pyridazines, pyrimidines, triazines and tetrazines which are available by routine chemical synthesis and are stable. The single and double bonds (i.e., -- or =) in such heterocycles are arranged based upon the heteroatoms present so that the heterocycle is aromatic (e.g., it is a heteroaryl group). The term heteroatom as applied herein refers to oxygen, nitrogen and sulfur. When the heteroaryl group comprises a five membered ring, W is preferably an electron withdrawing group, such as halogen, -CN, -CF₃, -NO₂, -COR⁷, -CO₂R⁶, -CONHR⁶, -SO₂NHR⁶, -

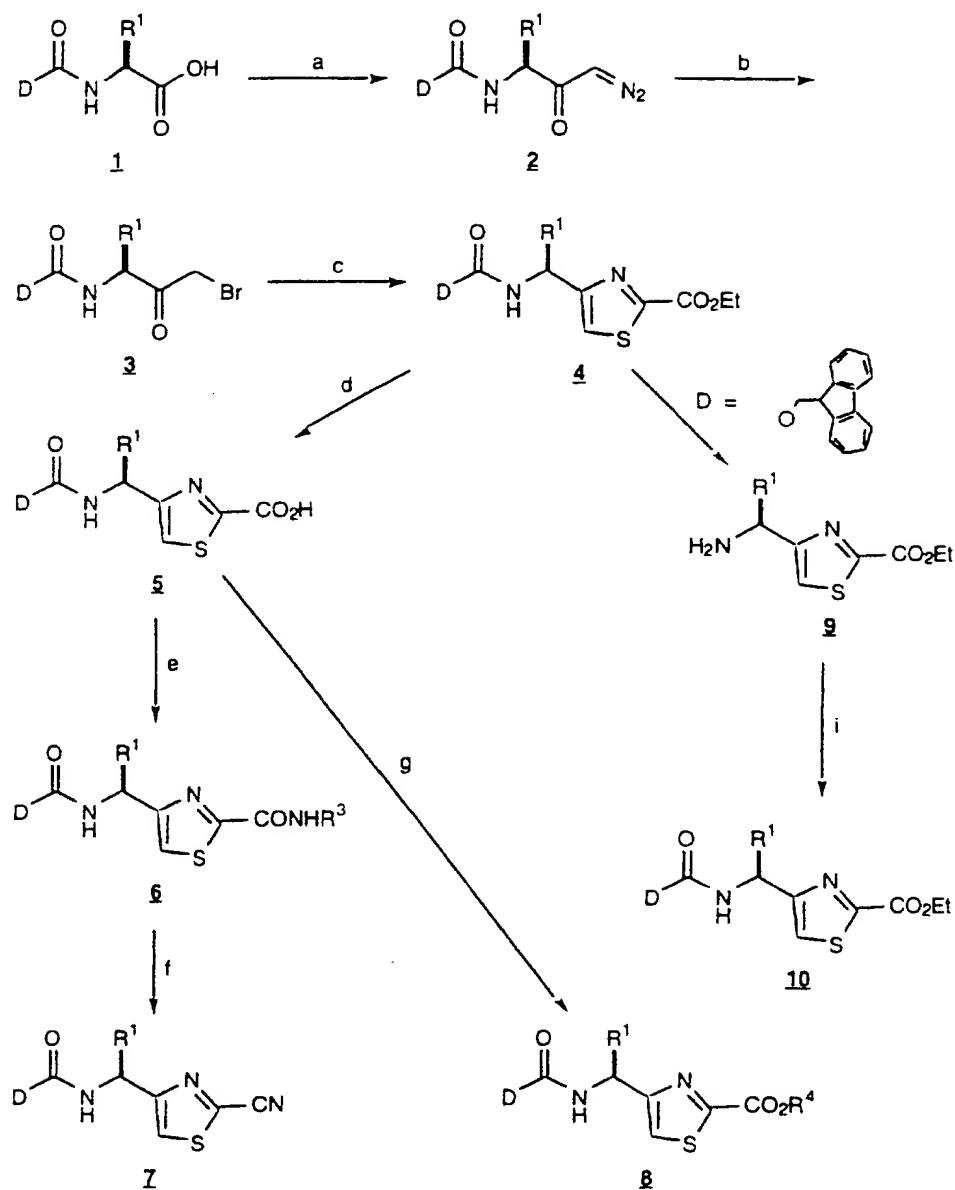
NHSO_2R^6 , -NHCOR^7 , -O-COR^6 , -SR^6 or NR^6R^6 , or a similar electron withdrawing substituent as known in the art.

Certain radical groups are abbreviated herein. t-Bu refers to the tertiary butyl radical, Boc refers to the t-butyloxycarbonyl radical, Fmoc refers to the
5 fluorenylmethoxycarbonyl radical, Ph refers to the phenyl radical, Cbz refers to the benzyloxycarbonyl radical.

Certain reagents are abbreviated herein. DCC refers to dicyclohexylcarbodiimide, DMAP is 2,6-dimethylaminopyridine, EDC refers to N-ethyl-N'-(dimethylaminopropyl)-carbodiimide. HOBT refers to 1-
10 hydroxybenzotriazole, DMF refers to dimethyl formamide, BOP refers to benzotriazol-1-yloxy-tris(dimethylamino)phosphonium hexafluorophosphate, DMAP is dimethylaminopyridine. Lawesson's reagent is 2,4-bis(4-methoxyphenyl)-1,3-dithia-2,4-diphosphetane-2,4-disulfide, NMM is N-methylmorpholine, TFA refers to trifluoroacetic acid, TFAA refers to trifluoroacetic anhydride and THF
15 refers to tetrahydrofuran. Jones reagent is a solution of chromium trioxide, water, and sulfuric acid well-known in the art.

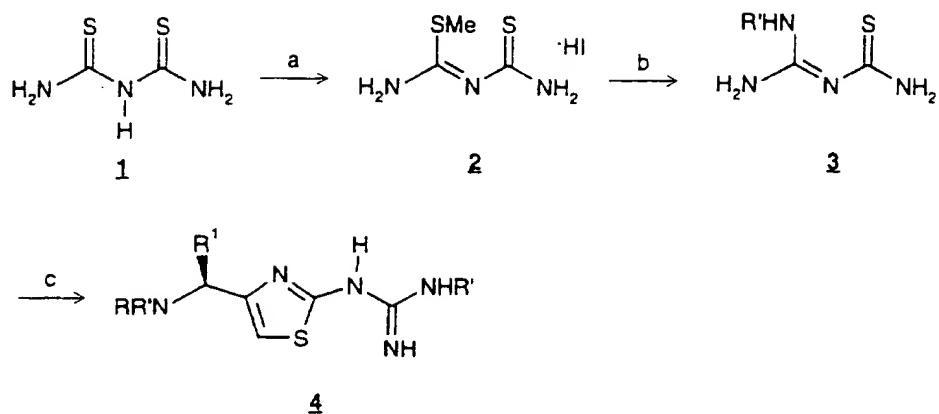
Compounds of formula (I) are prepared according to the methods detailed in Schemes 1-25.

Scheme 1



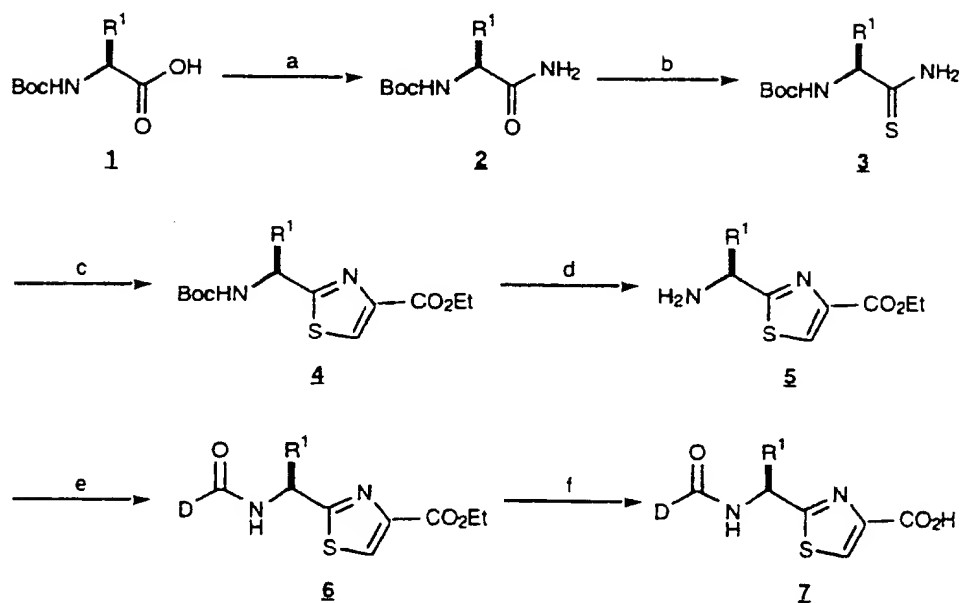
a) $i\text{-BuOCOC}l$, NMM, CH_2N_2 , EtOAc, Et_2O ; b) HBr , AcOH, EtOAc, Et_2O ; c) $\text{H}_2\text{NCSCOC}_2\text{Et}$, EtOH; d) NaOH , H_2O , THF; e) $i\text{-BuOCOC}l$, NMM, NH_2 , THF or BOP, Et_3N , RNH_2 , CH_2Cl_2 ; f) TFAA, pyridine, CH_2Cl_2 ; g) R^4OH , Boc_2O , Pyridine or R^4OH , EDCl, CH_2Cl_2 ; h) piperidine, DMF; i) BOP, Et_3N , $\text{D-CO}_2\text{H}$, CH_2Cl_2

Scheme 1A



5 a) MeI, THF; b) R'NH₂, *i*-PrOH; c) Bromomethyl ketone, EtOH

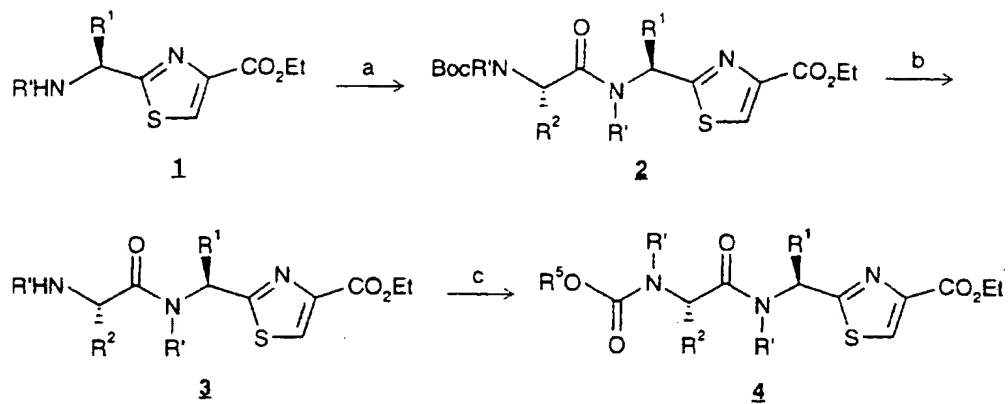
Scheme 2



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a) *i*-BuOCOC₂Cl, NMM, NH₃, THF; b) Lawesson's reagent, THF; c) BrCH₂COCOC₂Et, TFAA, Pyridine, CH₂Cl₂; d) TFA; e) DCO₂H, EDC·HCl, HOBT, Et₃N, DMF; f) NaOH, H₂O, THF

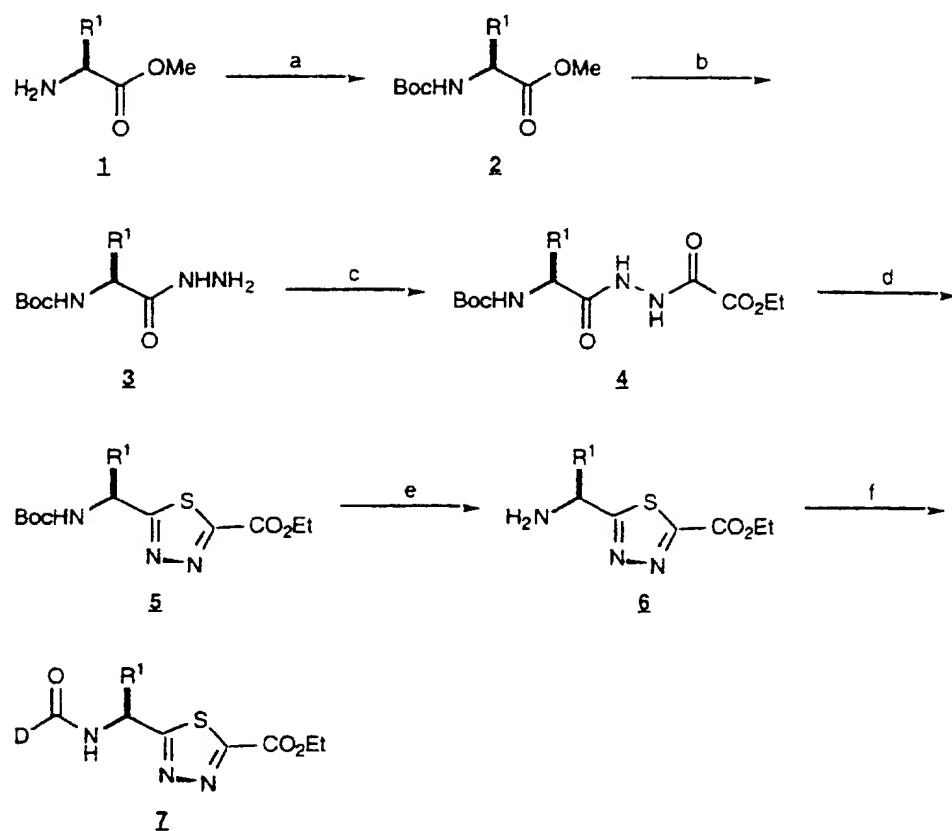
Scheme 2A



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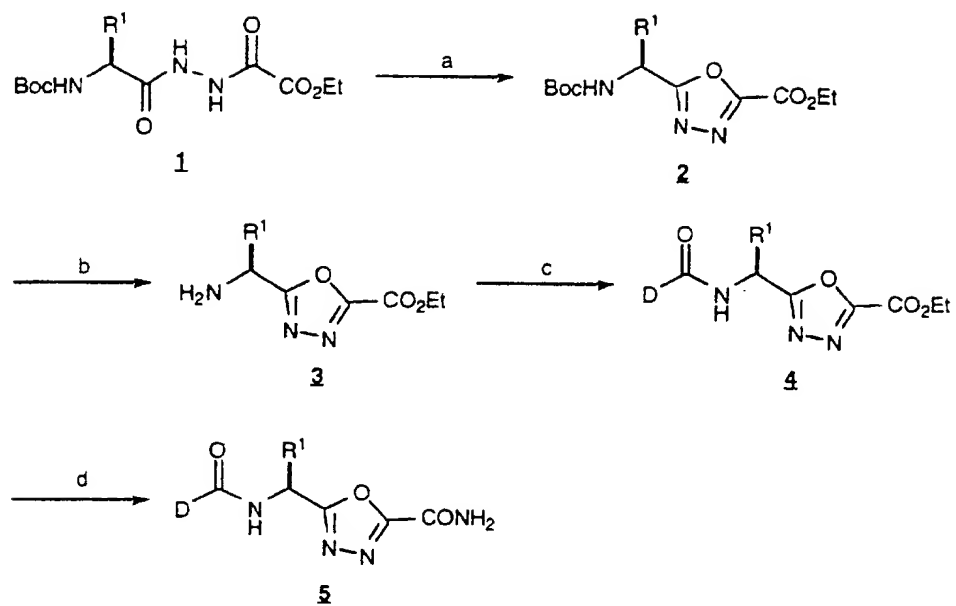
a) Boc-amino acid, EDC•HCl, 1-HOBT, DMF; b) TFA; c) R⁵OCOC(=O)Cl, *i*-Pr₂NEt

Scheme 3



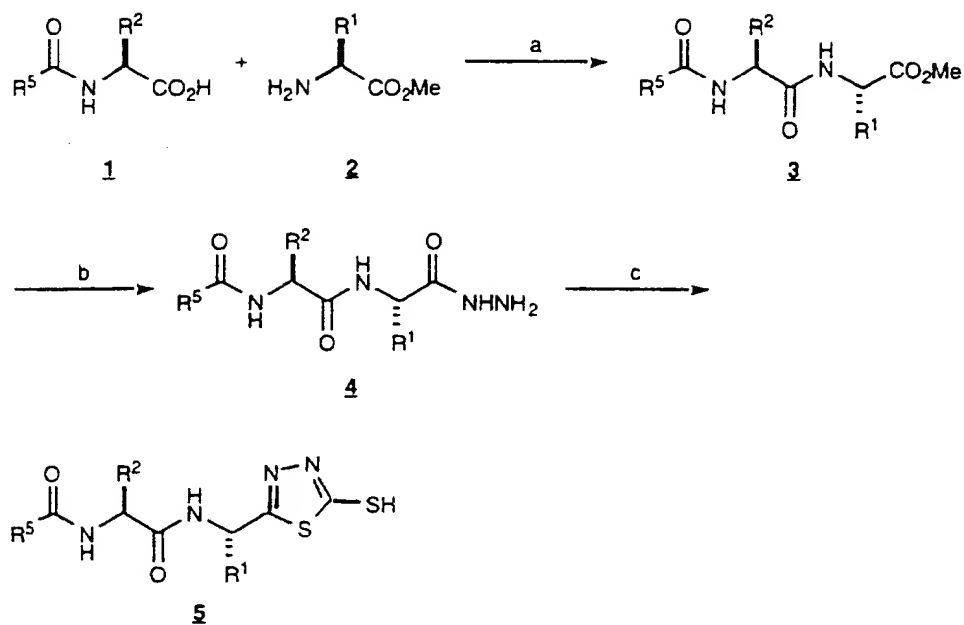
- a) Boc_2O , Et_3N , THF; b) hydrazine hydrate, MeOH; c) EtO_2CCOCl , Pyridine,
 5 CH_2Cl_2 ; d) Lawesson's reagent, toluene; e) TFA, CH_2Cl_2 ; f) DCO_2H ,
 $\text{EDC}\cdot\text{HCl}/\text{HOBT}$, Et_3N , DMF

Scheme 4



a) SOCl_2 , pyridine, Et_2O , toluene; b) TFA, CH_2Cl_2 ; c) DCO_2H , EDC•HCl/HOBT,
5 Et_3N , DMF; d) NH_3 , EtOH

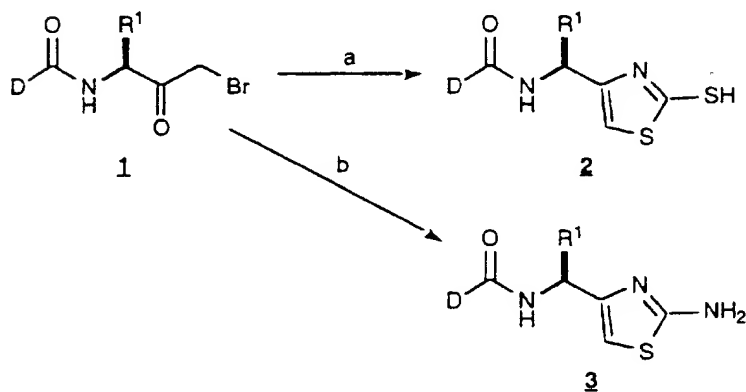
Scheme 5



a) EDC·HCl/HOBT, Et₃N, DMF; b) H₂NNH₂·H₂O, MeOH; c) CSCl₂, Et₃N, CHCl₃

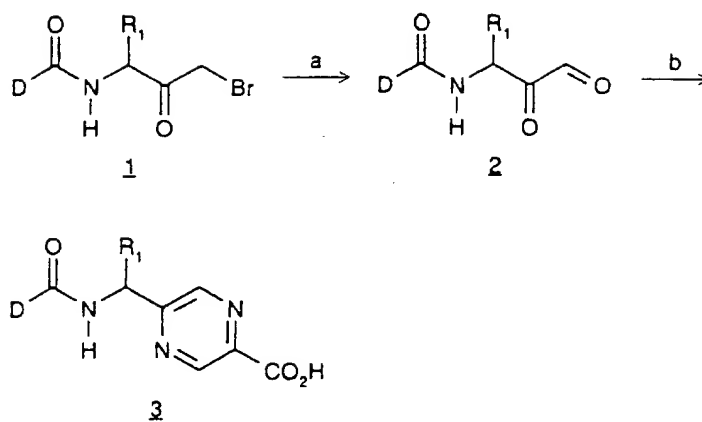
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Scheme 6



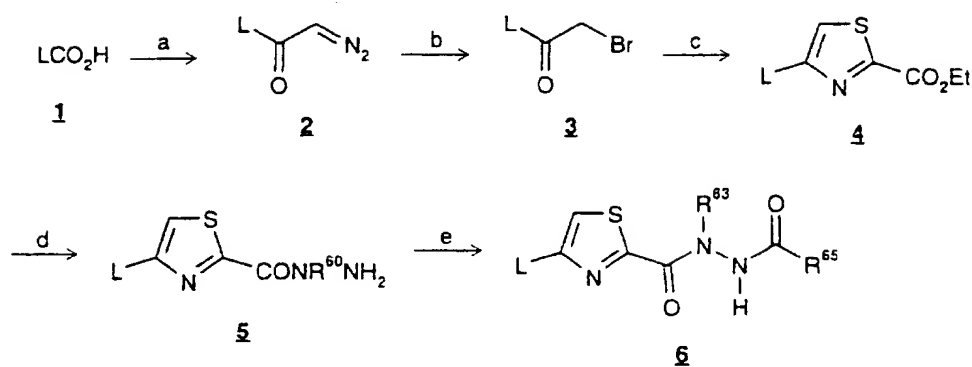
a) H₂NCS₂NH₄⁺, EtOH; b) H₂NCSNH₂, EtOH

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Scheme 7

a) Et_2NO ; b) $\text{H}_2\text{NCH}_2\text{CH}(\text{NH}_2)\text{CO}_2\text{H}$

5

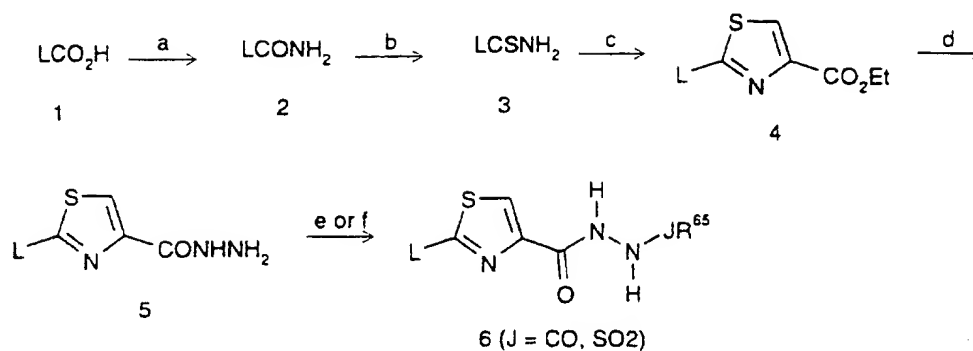
Scheme 8

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a) i. $i\text{-BuOCOCl}$, NMM, THF; ii. CH_2N_2 , Et_2O ; b) HBr , AcOH , Et_2O ; c) $\text{H}_2\text{NCSCO}_2\text{Et}$, EtOH ; d) $\text{R}^{63}\text{NHNH}_2$, EtOH ; e) $\text{R}^{65}\text{CO}_2\text{H}$, $\text{EDC}\cdot\text{HCl}$, 1-HOBT, DMF.

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Scheme 9

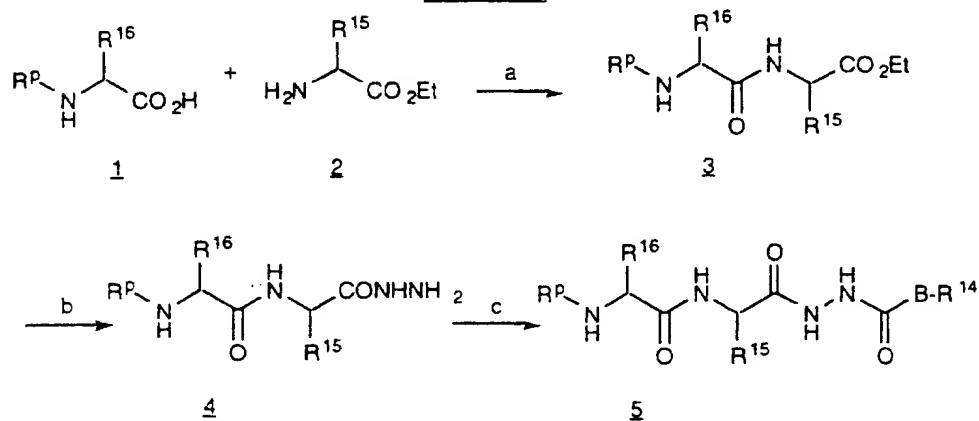


5

a) *i*-BuOCOC₂H₅Cl, NMM, NH₃, THF; b) Lawesson's reagent, THF; c) i. EtO₂CCOCH₂Br; ii. TFAA, Py, CH₂Cl₂; d) H₂NNH₂•H₂O, EtOH; e) R⁶⁵SO₂Cl, Py, CH₂Cl₂; f) R⁶⁵CO₂H, EDC•HCl, 1-HOBT, DMF.

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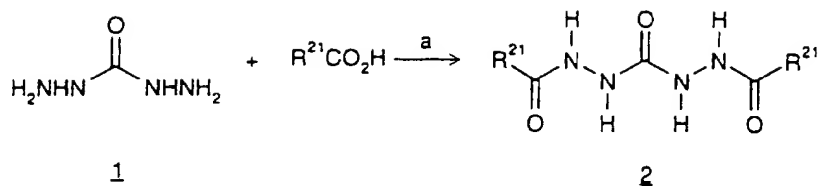
Scheme 10



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a) EDC•HCl, HOBT, DMF; b) H₂NNH₂•H₂O, EtOH; c) R¹⁴-B-CO₂H, EDC•HCl, HOBT, DMF

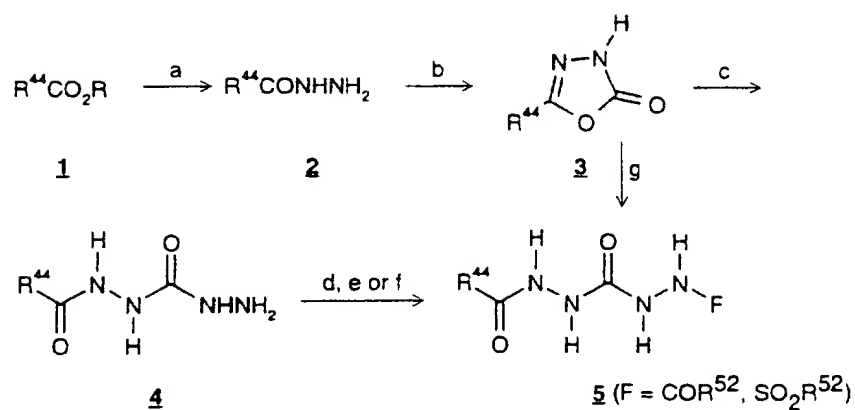
Scheme 11



a) EDC.HCl, 1-HOBT, DMF

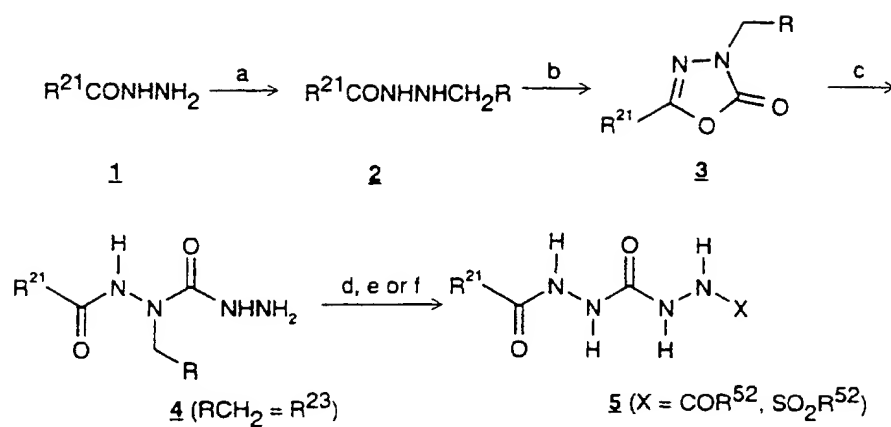
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Scheme 12



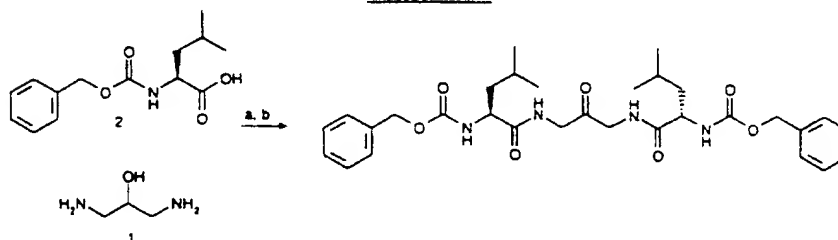
a) $\text{H}_2\text{NNH}_2 \cdot \text{H}_2\text{O}$, MeOH; b) Cl_2CO , PhMe; c) $\text{H}_2\text{NNH}_2 \cdot \text{H}_2\text{O}$, MeOH; d) $\text{R}^{49}\text{CO}_2\text{H}$, EDC.HCl, 1-HOBT, DMF; e) $\text{R}^{52}\text{SO}_2\text{Cl}$ or R^{52}COCl , pyridine, DMF; f) $\text{R}^{52}\text{CO}_2\text{COR}^{52}$; g) $\text{R}^{52}\text{CONR}^{51}\text{NH}_2$

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Scheme 12A

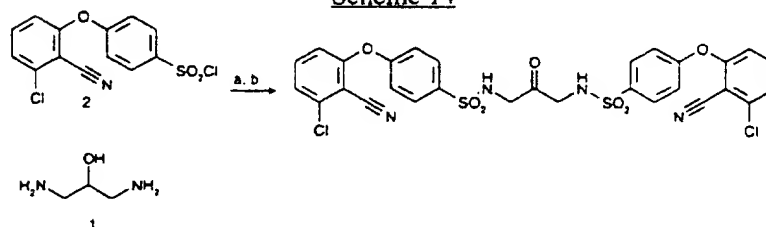
a) i. PhCHO, EtOH; ii. BH₃·THF; b) Cl₂CO, PhMe; c) H₂NNH₂·H₂O, MeOH; d) R⁵²CO₂H, EDC·HCl, 1-HOBT, DMF; e) R⁵²SO₂Cl or R⁵²COCl, pyridine, DMF; f) R⁵²CO₂COR⁵²

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Scheme 13

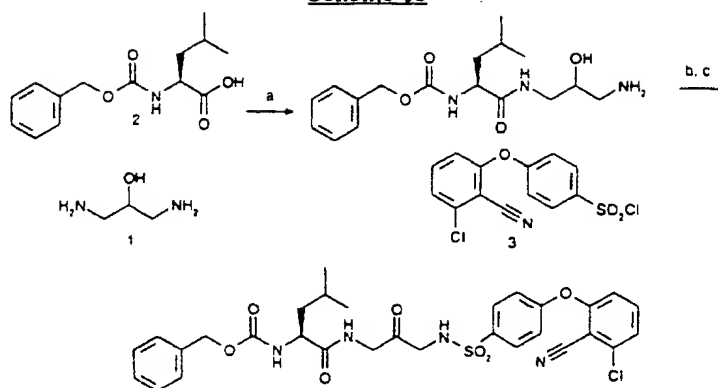
a) HBTU, NMM, DMF; b) Jones, acetone

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Scheme 14

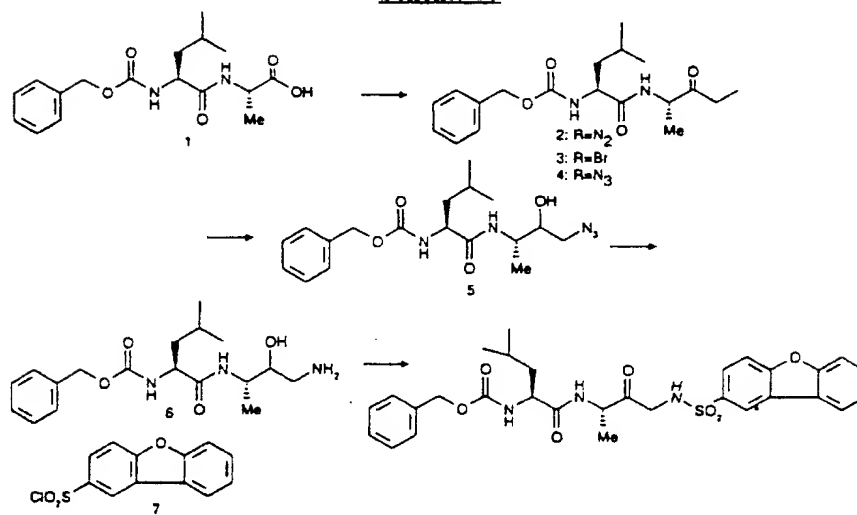
15 a) NMM, DMF; b) Jones, acetone

Scheme 15



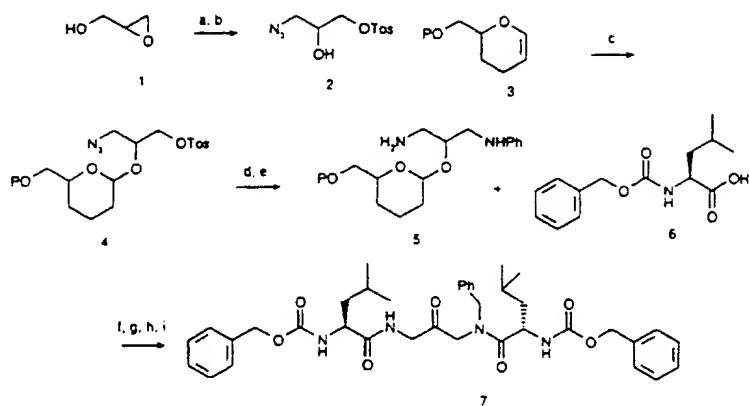
5 a) EDCI, HOBT, DMF; b) NMM, DMF, 3) Jones, acetone

Scheme 16



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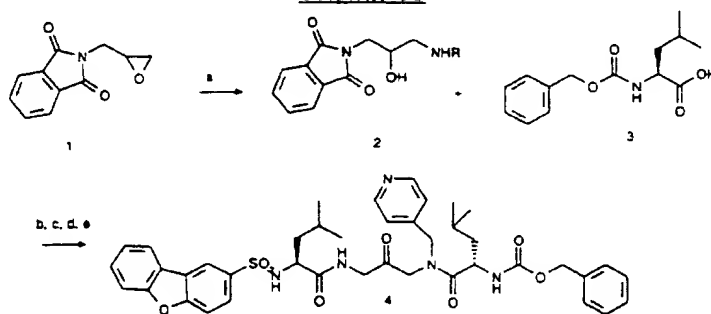
Scheme 17



- 5 a) NaN_3 , MeOH, H_2O ; b) Tosyl chloride, triethylamine, CH_2Cl_2 ; c) Ellman dihydropyran resin (3), PPTS, $\text{Cl}(\text{CH}_2)_2\text{Cl}$; d) PhCH_2NH_2 , toluene, 80 degrees C; e) HATU, N-methyl morpholine, NMP; f) $\text{HS}(\text{CH}_2)_3\text{SH}$, MeOH, Et_3N ; g) Cbz-leucine (6), HBTU, N-methyl morpholine, NMP; h) TFA, CH_2Cl_2 , Me_2S ; i) Jones reagent, acetone

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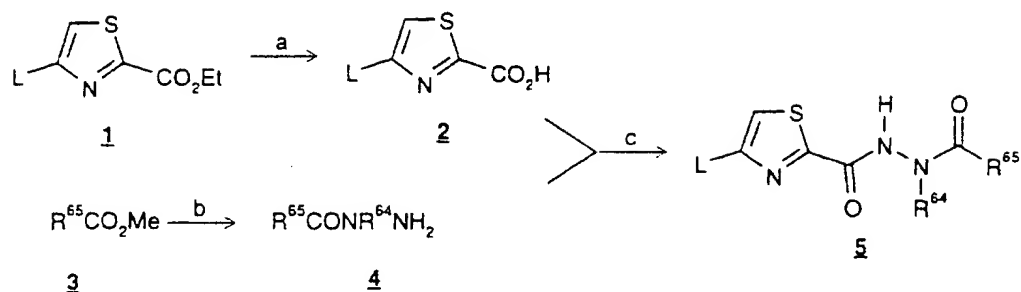
Scheme 18



- 15 a) 4-pyridyl methyl amine, isopropanol, reflux; b) Cbz-leucine, HBTU, N-methyl morpholine, DMF; c) hydrazine, MeOH, reflux; d) 2-dibenzofuransulfonyl chloride, N-methyl morpholine, DMF; e) Jones reagent, acetone

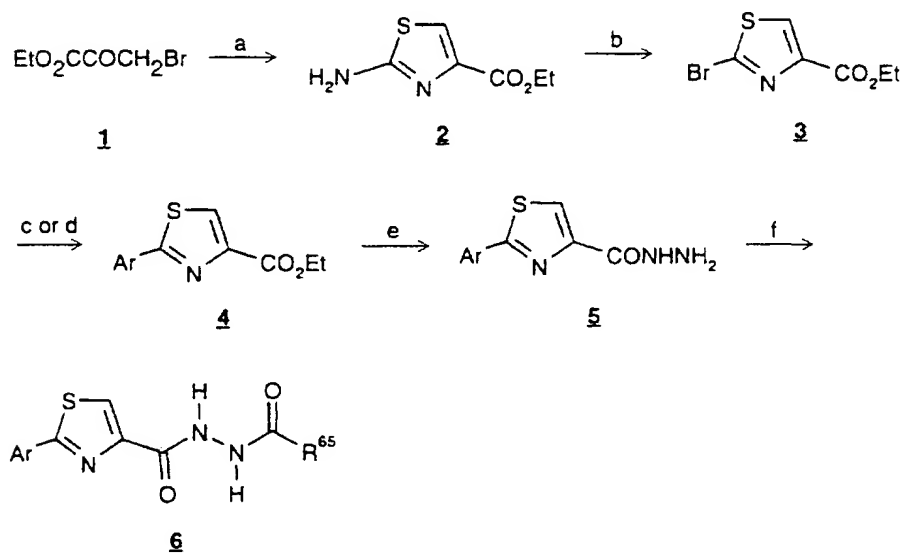
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Scheme 19



5 a) KOH, MeOH/H₂O; b) R⁶⁶NHNH₂, EtOH; c) EDC•HCl, 1-HOBT, DMF

Scheme 20

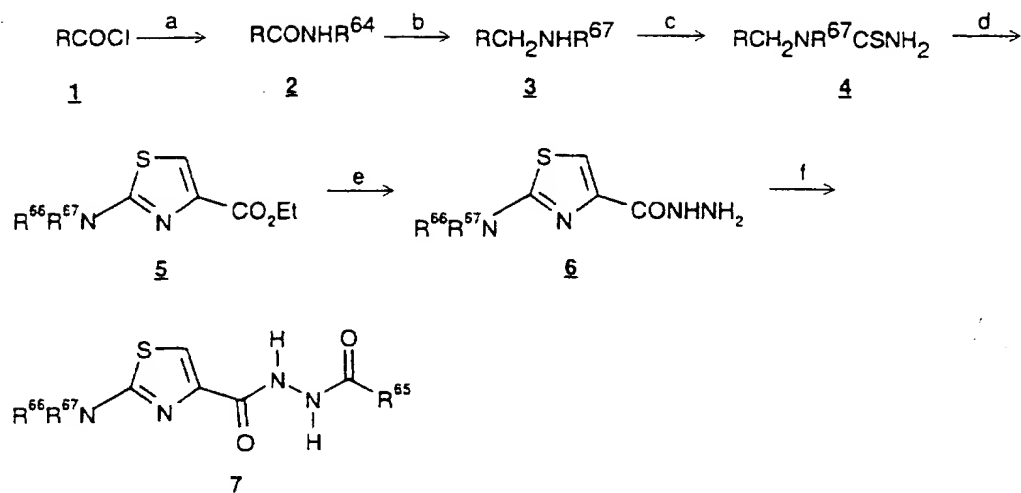


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a) Thiourea, EtOH; b) i. NaNO₂, 16% aqueous HBr; ii. CuBr, 16% aqueous HBr; iii. HBr (cat.), EtOH; c) ArB(OH)₂, Pd(PPh₃)₄, CsF, DME; d) ArSnMe₃, Pd(PPh₃)₄, PhMe; e) H₂NNH₂•H₂O, EtOH; f) R⁶⁵CO₂H, EDC•HCl, 1-HOBT, DMF.

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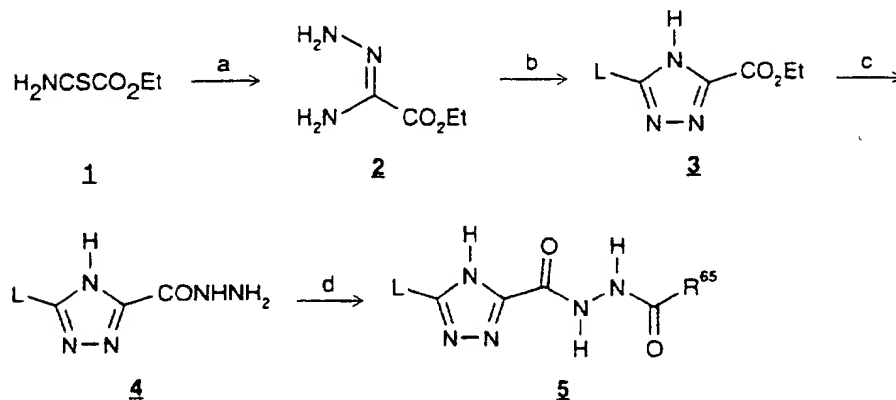
Scheme 21



- 5 a) R^{67}NH_2 , Py, CH_2Cl_2 ; b) LiAlH_4 , THF; c) i. Cl_2CS , Py, CH_2Cl_2 ; ii. NH_3 , MeOH or I. PhCONCS , CHCl_3 ; ii. K_2CO_3 , MeOH, H_2O ; d) $\text{EtO}_2\text{CCOCH}_2\text{Br}$, EtOH; e) $\text{H}_2\text{NNH}_2 \cdot \text{H}_2\text{O}$, EtOH; e) $\text{R}^{65}\text{CO}_2\text{H}$, $\text{EDC} \cdot \text{HCl}$, 1-HOBT, DMF.

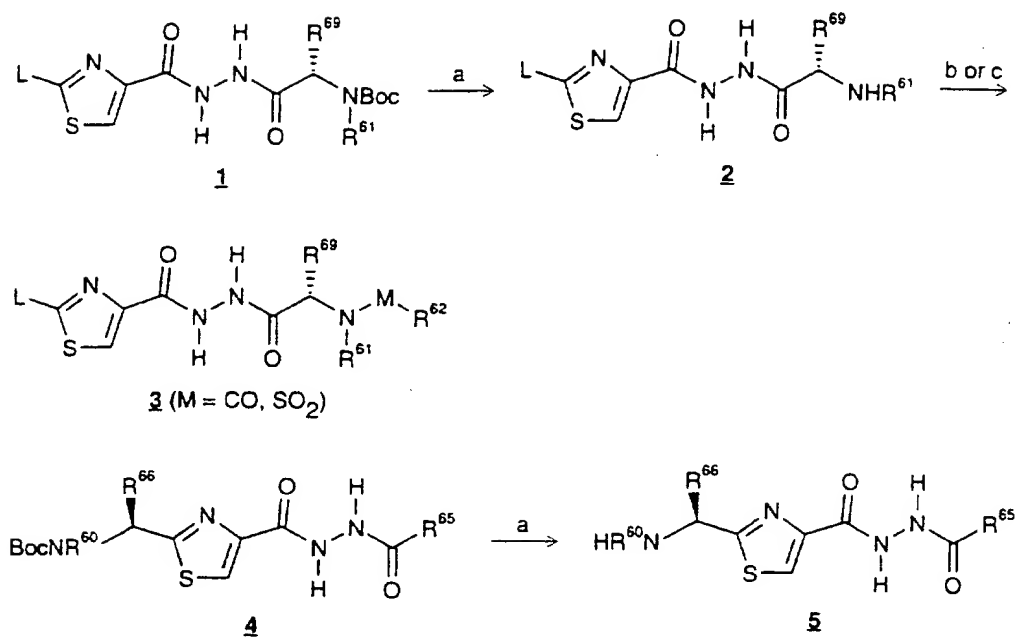
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Scheme 22



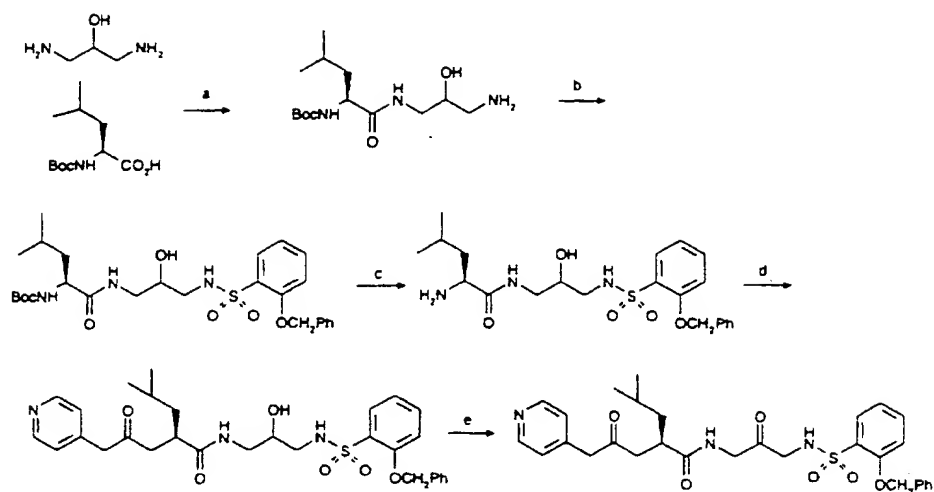
- a) $\text{H}_2\text{NNH}_2 \cdot \text{H}_2\text{O}$, EtOH; b) $\text{LCO}_2\text{CO}_2i\text{-Bu}$, 200 °C; c) $\text{H}_2\text{NNH}_2 \cdot \text{H}_2\text{O}$, EtOH; d) $\text{R}^{65}\text{CO}_2\text{H}$, $\text{EDC} \cdot \text{HCl}$, 1-HOBT, DMF

Scheme 23



5 a) TFA; b) $\text{R}^{62}\text{CO}_2\text{H}$, EDC•HCl, 1-HOBT, DMF; c) $\text{R}^{62}\text{SO}_2\text{Cl}$, *i*-Pr₂NEt

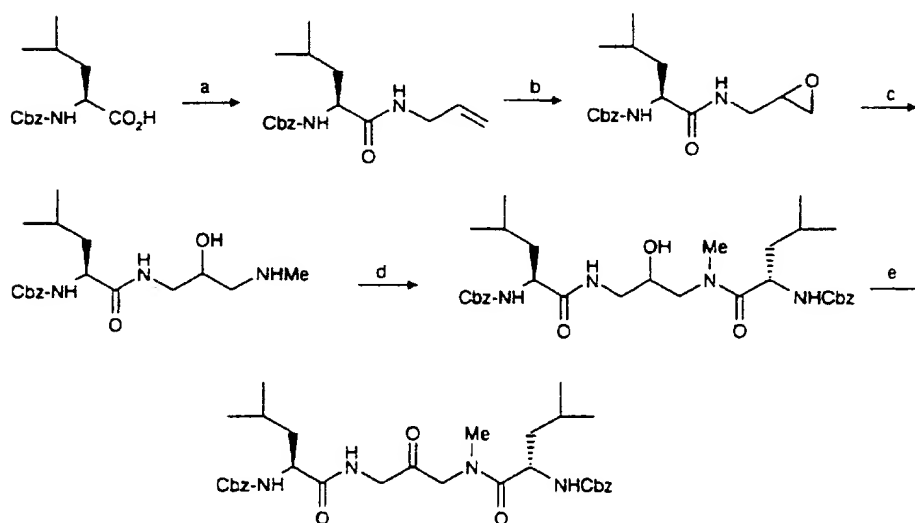
Scheme 24



- 5 a) EDCI, DMF; b) 2-PhCH₂OPhSO₂Cl, NMM, DMF; c) TFA, DCM; d) 4-pyridyl acetic acid, HBTU, NMM, DMF; e) Jones

Scheme 25

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- a) HBTU, NMM, DMF, allyl amine; b) mCPBA, DCM; c) MeNH₂, isopropanol, 70 °C; d) Cbz-leucine, EDCI, DMF; e) Jones, acetone

In another aspect, the present invention provides a novel cysteine protease in crystalline form, as defined by the positions in Table I herein.

In still another aspect, the present invention provides a novel protease
5 composition characterized by a three dimensional catalytic site formed by the atoms of the amino acid residues listed in Table XXIX herein.

The three dimensional (3D) structure of the instant protease reveals that human cathepsin K is highly homologous to other known cysteine proteinases of the papain family. Cathepsin-K folds into two subdomains separated by the active site
10 cleft, a characteristic of the papain family of cysteine proteases. The overall fold of cathepsin K is very similar to that of papain and actinidin. There is an insertion of one additional residue in cathepsin K at residue alanine 79 compared to papain. This insertion is easily accommodated in the turn at the carboxy terminal end of the helix formed by residues methionine 68-lysine 77 of cathepsin K. There is a different
15 conformation for the backbone atoms of residues asparagine 99 to lysine 103 at the surface of cathepsin K compared to that in papain. Other differences in the backbone conformations between cathepsin K and papain are: a two residue insertion in loop residues 126-127, a two residue insertion at residue aspartate 152, the insertion of 4 residues at glutamine 172 and a difference in the conformation of
20 the loop around residue lysine 200. There are many more differences in the structure of human cathepsin K and human cathepsin B, however, the secondary structure is preserved well between these two enzymes.

Listed in Figure 1 are the known amino acid sequences for the papain
superfamily of cysteine proteases cathepsin K, cathepsin S, cathepsin L, papain,
25 actinidin, cathepsin H and cathepsin B, aligned to illustrate the homologies there between.

According to the present invention the crystal structure of human
cathepsin K has been determined in the absence of inhibitor and in complex with
nine separate inhibitors at resolutions from 3.0 to 2.2 Ångstroms. The structures
30 were determined using the method of molecular replacement and refined to R_c values ranging from 0.190-0.267 with the exception of the enzyme in the absence of inhibitor which was not refined.

Further refinement of the atomic coordinates will change the numbers in
Table I. Refinement of the crystal structure from another crystal form will result in a
35 new set of coordinates, determination of the crystal structure of another cysteine

protease will also result in different set of numbers for coordinates in Table I which has an experimental error of approximately 0.4 Ångstroms. Also for example, the amino acid sequence of the cysteine proteases can be varied by mutation derivatization or by use of a different source of the protein.

5 Human cathepsin K contains 215 amino acids and the model of the enzyme provided herein is represented by all 215 residues.

The cathepsin K crystal structure reveals an active site that is heretofor unknown and comprises a distinct three dimensional arrangement of atoms.

Table I discloses the protein coordinates of cathepsin K. These data are
10 reported for the crystal structures described herein. The data are reported in Ångstroms with reference to an orthogonal coordinate system in standard format, illustrating the atom, i.e., nitrogen, oxygen, carbon, sulfur (at α , β , γ , δ , or ϵ , positions in the amino acid residues); the amino acid residue in which the atom is located with amino acid number, and the coordinates X, Y and Z in Angstroms (Å)
15 from the crystal structure. Note that each atom in the active site and the entire structure has a unique position in the crystal. The data also report the B or Temperature Factor values, which indicate the degree of thermal motion of the atom in root mean square displacement measurements (\AA^2). Figure 2 illustrates the cathepsin K structure of the invention, including the active site.

20 The active site of cathepsin K bound to E-64 is shown in Figure 3. The conformation of E-64 bound to cathepsin K resembles that seen in the published structures of the papain-E-64 complex (Varughese, K.I., *Biochemistry* 28, 1330-1332 (1989)) and actinidin-E-64 Varughese, K.I., *Biochemistry* 31, 5172-5176 (1992)). The covalent bond between the sulfur of cysteine 25 and the carbon C2 of the inhibitor is very clear in the electron density. Differences in the sidechain atoms lining the active site pockets on the enzyme of the various members of the papain family of cysteine proteases give rise to different interactions between the atoms of E-64 and the protein in these structures. In cathepsin K, the isobutyl atoms of the leucine lie well buried in the hydrophobic pocket formed by the side chain atoms of
30 the cathepsin K residues leucine 160, alanine 134 and methionine 68 shielding these atoms of E-64 from solvent. In papain the leucyl side chain atoms of E-64 do not penetrate as deeply into this hydrophobic pocket. Another pocket of cathepsin K is occupied by the guanidinium atoms of E-64. A hydrogen bond forms between N4 of E-64 and the backbone carbonyl oxygen of glutamate 59 and the OD2 oxygen of aspartate 61. The carboxylate oxygen of aspartate 61 also makes a hydrogen bond
35

with the N3 atom of E-64. The sidechain atoms of aspartate 61 lie at the entrance to this pocket in cathepsin K. These interactions are not possible in papain because the corresponding residue in papain is tyrosine 61 which blocks access. The carboxylate oxygens of E-64 make hydrogen bonding interactions with the ND1 atom of histidine 162 and the NE2 atom of glutamine 19. These interactions are also seen in papain and actinidin. The atoms of E-64 do not penetrate the complete region of the enzyme active site. As in papain, the backbone nitrogen atoms of residue glycine 66 in cathepsin K makes a hydrogen bond with the carbonyl oxygen atom O4 of the E-64. Also, the carbonyl oxygen of glycine 66 of cathepsin K forms a hydrogen bond with N2 of E-64. A portion of the regions of the active site are very similar in conformation in cathepsin K, papain and actinidin. A comparison of the active site of cathepsin K and cathepsin B reveals many more differences than observed in comparing papain or actinidin to cathepsin K. A portion of the active site of cathepsin B differs significantly from the corresponding portion of the active site in cathepsin K. The presence of the loop glutamate 107 - proline 116 in human cathepsin B is presumed responsible for the dipeptidyl carboxypeptidase activity of this enzyme and has no equivalent in cathepsin K, papain or actinidin. This loop makes this region of the active site of cathepsin B much smaller than in the other members of this papain family of cysteine proteases including cathepsin K. Despite the differences between the active sites of human cathepsin B and cathepsin K, the active site cysteine residues are almost exactly superimposed by an alignment of structurally homologous alpha carbon atoms in cathepsin B and cathepsin K. Differences in the hydrophobic pocket near leucine 160 in cathepsin K are also evident in cathepsin B. The residues forming this pocket are replaced by proline 78 in place of methionine 68 in cathepsin K and glutamate 243 in cathepsin B is structurally equivalent to leucine 160 in cathepsin K. Interestingly, the residues whose sidechain atoms form hydrogen bonds to the E-64 inhibitor in cathepsin K, namely histidine 162, glutamine 19 and aspartate 61, have structurally homologous residues in cathepsin B, namely histidine 197, glutamine 23 and aspartate 67 respectively.

Specific interactions of certain inhibitors of the present invention at the active site of cathepsin K are detailed hereinbelow.

3 (S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone makes hydrophobic contacts with the enzyme residues indole ring of tryptophan 184 and the sidechain atom CG of glutamine 19. Oxygen O26 forms a

bifurcated hydrogen bond with the amide nitrogen of cysteine 25 and the NE2 atom of glutamine 19. The active site nucleophilic sulfur of residue cysteine 25 is covalently linked to carbon C25 of the inhibitor, which adopts a tetrahedral conformation.

5 Bis-(Cbz-leuciny)-1,3-diamino-propan-2-one exhibits the same interaction as 3 (S)-3-[(N-benzyloxycarbonyl)-L-leuciny]amino-5-methyl-1-(1-propoxy)-2-hexanone; carbon C21 of this inhibitor is covalently linked to SG of cysteine 25. The isopropyl atoms CC34, C35, C36 and C37 of the inhibitor form hydrophobic interactions with the sidechain atoms of residues on the enzyme surface, which form
10 a hydrophobic pocket. This pocket is formed by atoms from methionine 68, leucine 209, alanine 163 and alanine 134 and portions of tyrosine 67.

2,2'-N,N'-bis-benzyloxycarbonyl-L-leuciny]carbohydrazide has interactions similar to bis-(Cbz-leuciny)-1,3-diamino-propan-2-one and, in addition, the atoms C23-29 of the inhibitor CBZ group make an edge-face stacking interaction with the
15 phenol ring of tyrosine 67. Inhibitor atom C21 is covalently bound the enzyme.

The sulfur atom of (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leuciny]hydrazide contacts the ND1 atom of histidine 163 and the indole ring of tryptophan 184. Carbon C22 is covalently attached to SG of cysteine 25.

20 The CBZ atoms C20-26 of 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leuciny)]carbohydrazide interact with the sidechain atoms of leucine 160. Carbon C19 is covalently attached to SG of cysteine 25.

Cathepsin K binds selectively one stereoisomer of 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone. Carbon C22 is covalently attached to SG of cysteine 25. Atoms C14
25 and C15 of the inhibitor 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone form hydrophobic contacts with the sidechain atoms of glutamine 143 and asparagine 161 and the mainchain of alanine 137 and serine 138.

30 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone interacts in a similar manner to 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone. Again one stereoisomer is bound. Carbon C17 is covalently attached to SG of cysteine 25. The interaction of 4-[N-
35 [(phenylmethoxy)carbonyl]-L-leucyl]-1-N[(methyl)-L-leucyl]-3-pyrrolidinone is

the same as for 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone, except carbon C22 is covalently attached to SG of cysteine 25.

Atom O24 of 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one forms a hydrogen bond interaction with the amide NH of glycine 66. Carbon C19 is covalently attached to SG of cysteine 25.

In summary, all inhibitors exhibit an aromatic interaction with atoms of the indole of Tryptophan 184. Isopropyl atoms C12-15 of 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide and (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide make hydrophobic contacts with main chain atoms of residues glutamine 21, cysteine 22 and glycine 23. The NE2 atom of glutamine 19 is able to donate a hydrogen bond to oxygen atom 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide:O22, 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one:O20, 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide:O20, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:O23, bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one:O22, 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone:O26, 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:O42, (1S, 2'R)-N-2-[[[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-2'-(benzyloxycarbonyl)amino-4'-methylpenanoylhydrazide:O23, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl]-3-pyrrolidinone:O23. The backbone amide nitrogen of glycine 66 donates a hydrogen bond to 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide:O39, 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one:O24, 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leucinyl)]carbohydrazide:O37, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:O40, bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one:O39, (1S, 2'R)-N-2-[[[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-2'-(benzyloxycarbonyl)amino-4'-methylpenanoylhydrazide:O40, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl]-3-pyrrolidinone:O31. The hydrophobic pocket lined with atoms from residues methionine 68, leucine 209, alanine 163 and alanine 134 and portions

of tyrosine 67 interact with the isopropyl atoms; bis-(Cbz-leuciny)-1,3-diamino-propan-2-one:C34-37, 2,2'-N,N'-bis-benzoyloxycarbonyl-L-leuciny-carbohydrazide: C34-37, (1S)-N-[2-[(1-benzoyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzoyloxycarbonyl-L-leuciny)hydrazide; :C35-38, 2-[N-(3-benzoyloxybenzoyl)]-2'-[N'-(N-benzoyloxycarbonyl-L-leuciny)]carbohydrazide:C32-35, 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:C35-38, 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone:C19-22, 1-N-(N-imidazole acetyl-leuciny)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one:C26-29. All inhibitors except 3(S)-3-[(N-benzoyloxycarbonyl)-L-leuciny]amino-5-methyl-1-(1-propoxy)-2-hexanone and 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl]-3-pyrrolidinone have aromatic groups that interact with tyrosine 67 on the protein. All inhibitors are covalently linked to the cysteine 25 SG atom through an inhibitor carbon atom.

15 The crystal structure of the protease of the present invention reveals the three dimensional structure of novel active site formed by the atoms of the amino acid residues listed in Table XXIX.

 This structure is clearly useful in the structure-based design of protease inhibitors, which may be used as therapeutic agents against diseases in which inhibition of bone resorption is indicated. The discovery of the novel cathepsin K catalytic site permits the design of potent, highly selective protease inhibitors.

20 Another aspect of this invention involves a method for identifying inhibitors of cathepsin K characterized by the crystal structure and novel active site described herein, and the inhibitors themselves. The novel protease crystal structure of the invention permits the identification of inhibitors of protease activity. Such inhibitors may bind to all or a portion of the active site of cathepsin K; or even be competitive or non-competitive inhibitors. Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block protease activity.

30 One design approach is to probe the cathepsin K of the invention with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate cathepsin K inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks.

Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their cathepsin K inhibitor activity.

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to or with cathepsin K. Thus, the time-dependent
5 analysis of structural changes in cathepsin K during its interaction with other molecules is permitted. The reaction intermediates of cathepsin K can also be deduced from the reaction product in co-complex with cathepsin K. Such information is useful to design improved analogues of known cysteine protease
10 inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the cathepsin K enzyme and cathepsin K inhibitor co-complex. This provides a novel route for designing cathepsin K inhibitors with both high specificity and stability.

Another approach made possible by this invention, is to screen
15 computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the cathepsin K enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity [R. L. DesJarlais et al., J. Med. Chem. 31:722-729 (1988)] or by estimated interaction energy [E. C. Meng et al, J. Comp. Chem.,
20 13:505-524 (1992)].

Because cathepsin K may crystallize in more than one crystal form, the structure coordinates of cathepsin K, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of cathepsin K. They may also be used to solve the structure of cathepsin K mutants,
25 cathepsin K co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of cathepsin K.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of cathepsin K, a cathepsin K mutant, or a cathepsin K co-complex, or
30 the crystal of some other protein with significant amino acid sequence homology to any functional domain of cathepsin K, may be determined using the cathepsin K structure coordinates of this invention as provided in Table I. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Thus, the cathepsin K structure provided herein permits the screening of known molecules and/or the designing of new molecules which bind to the protease structure, particularly at the active site, via the use of computerized evaluation systems. For example, computer modeling systems are available in which the
5 sequence of the protease, and the protease structure (i.e., atomic coordinates of cathepsin K and/or the atomic coordinate of the active site cavity, bond angles, dihedral angles, distances between atoms in the active site region, etc. as provided by Table I may be input. Thus, a machine readable medium may be encoded with data representing the coordinates of Table I in this process. The computer then
10 generates structural details of the site into which a test compound should bind, thereby enabling the determination of the complementary structural details of said test compound.

More particularly, the design of compounds that bind to or inhibit cathepsin K according to this invention generally involves consideration of two factors. First,
15 the compound must be capable of physically and structurally associating with cathepsin K. Non-covalent molecular interactions important in the association of cathepsin K with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it
20 to associate with cathepsin K. Although certain portions of the compound will not directly participate in this association with cathepsin K, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or
25 compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of cathepsin K, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with cathepsin K.

The potential inhibitory or binding effect of a chemical compound with
30 cathepsin K may be estimated prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and cathepsin K, synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for

its ability to bind to cathepsin K in a suitable assay. In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of cathepsin K may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of cathepsin K.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with cathepsin K and more particularly with the individual binding pockets of the cathepsin K active site or accessory binding site. This process may begin by visual inspection of, for example, the active site on the computer screen based on the cathepsin K coordinates in Table I. Selected fragments or chemical entities may then be positioned on cathepsin K. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

- GRID [P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., **28**:849-857 (1985)]. GRID is available from Oxford University, Oxford, UK.
- MCSS [A. Miranker and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method", Proteins: Structure, Function and Genetics, **11**:29-34 (1991)]. MCSS is available from Molecular Simulations, Burlington, MA.
- AUTODOCK [D. S. Goodsell and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, **8**:195-202 (1990)]. AUTODOCK is available from Scripps Research Institute, La Jolla, CA.
- DOCK [I. D. Kuntz et al, "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., **161**:269-288 (1982)]. DOCK is available from University of California, San Francisco, CA.

Additional commercially available computer databases for small molecular compounds includes Cambridge Structural Database and Fine Chemical Database, for a review see Rusinko, A., Chem. Des. Auto. News **8**, 44-47 (1993).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of cathepsin K. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

- CAVEAT [P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems, Special Pub., Royal Chem. Soc. 78, pp. 182-196 (1989)]. CAVEAT is available from the University of California, Berkeley, CA.

- 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35:2145-2154 (1992).

- HOOK (available from Molecular Simulations, Burlington, MA).

Instead of proceeding to build a cathepsin K inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other type of binding compounds may be designed as a whole or "*de novo*" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include:

- LUDI [H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6:61-78 (1992)]. LUDI is available from Biosym Technologies, San Diego, CA.

- LEGEND [Y. Nishibata and A. Itai, Tetrahedron, 47:8985 (1991)]. LEGEND is available from Molecular Simulations, Burlington, MA.

- LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al, "Molecular Modeling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33:883-894 (1990). See also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2:202-210 (1992). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous

methods and techniques are known in the art for performing this step, any of which may be used. See, e.g., P.S. Farmer, Drug Design, Ariens, E.J., ed., Vol. 10, pp 119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; C. Verlinde, Structure, 2:577-587 (1994); and I. D. Kuntz, Science, 5 257:1078-1082 (1992). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Thus, using these computer evaluation systems, a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many 10 compounds is effectively eliminated.

Once identified by the modeling techniques, the protease inhibitor may be tested for bioactivity using standard techniques. For example, structure of the invention may be used in binding assays using conventional formats to screen inhibitors. Suitable assays for use herein include, but are not limited to, the enzyme- 15 linked immunosorbent assay (ELISA), or a fluorescence quench assay. See, for example, the cathepsin K activity assay of Example 2 below. Other assay formats may be used; these assay formats are not a limitation on the present invention.

In another aspect, the protease structure of the invention permit the design and identification of synthetic compounds and/or other molecules which have a 20 shape complimentary to the conformation of the protease active site of the invention.

Using known computer systems, the coordinates of the protease structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the protease of the invention. Subsequently, suitable candidates identified as above may 25 be screened for the desired protease inhibitory bioactivity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block cathepsin K activity.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention which is defined by the appended 30 claims.

EXAMPLE 1: Analysis of the Structure of Cathepsin K

A. Expression, Purification and Crystallization

Cathepsin K (see Fig. 1) was expressed and purified as described in 35 Bossard, M. J., et al., *J. Biol. Chem.* **271**, 12517-12524 (1996).

Crystals of cathepsin K were grown by vapor diffusion in hanging drops from a solution of 30% PEG 8000, 0.1 M Na⁺/K⁺ phosphate at pH 4.5 containing 0.2M Li₂SO₄. Crystals of the complex are tetragonal, space group P4₃2₁2, with cell constants of a=57.7 Ångstroms and c=131.1 Ångstroms. The crystals contain
5 one molecule in the asymmetric unit and contain 36 % solvent with a V_m value of 2.3 Å³/Dalton. The structure was determined by molecular replacement using X-PLOR [Brunger, A.T., et al., *Science*, **235**, 458-460 (1987)]. The starting model consisted of the protein atoms from the cathepsin K E-64 complex structure described herein.

10 **B. Model Building and Refinement**

Using the three-dimensional electron density map obtained from above, the polypeptide chain of the cathepsin K can be traced without ambiguity. All 215 residues with side chains were built using the 3-D computer graphics program FRODO [Jones, T.A., *J. Appl. Crystallogr.*, **11**, 268-272 (1978)]. Each of
15 these 215 amino acids residues was manually positioned in its electron density, allowing for a unique position for each atom in cathepsin K in which each position is defined by a unique set of atomic coordinates (X,Y,Z) as shown in Table I. Starting with these atomic coordinates, a diffraction pattern was calculated and compared to the experimental data. The difference between the calculated and experimentally
20 determined diffraction patterns was monitored by the value of R_c. The refinement (using X-PLOR) of the structural model necessitates adjustments of atomic positions to minimize the R-factor, where a value of below 20% is typical for a good quality protein structure and a value of higher than 25% usually indicates the need of further refinement.

25

EXAMPLE 2: Assays

Determination of cathepsin K proteolytic catalytic activity

All assays for cathepsin K were carried out with human recombinant enzyme. Standard assay conditions for the determination of kinetic constants used a
30 fluorogenic peptide substrate, typically Cbz-Phe-Arg-AMC, and were determined in 100 mM Na acetate at pH 5.5 containing 20 mM cysteine and 5 mM EDTA. Stock substrate solutions were prepared at concentrations of 10 or 20 mM in DMSO with 20 uM final substrate concentration in the assays. All assays contained 10% DMSO. Independent experiments found that this level of DMSO had no effect on enzyme
35 activity or kinetic constants. All assays were conducted at ambient temperature.

Product fluorescence (excitation at 360 nM; emission at 460 nM) was monitored with a Perceptive Biosystems Cytofluor II fluorescent plate reader. Product progress curves were generated over 20 to 30 minutes following formation of AMC product.

5 Inhibition studies

Potential inhibitors were evaluated using the progress curve method. Assays were carried out in the presence of variable concentrations of test compound. Reactions were initiated by addition of enzyme to buffered solutions of inhibitor and substrate. Data analysis was conducted according to one of two procedures depending on the appearance of the progress curves in the presence of inhibitors. For those compounds whose progress curves were linear, apparent inhibition constants ($K_{i,app}$) were calculated according to equation 1 (Brandt *et al.*, *Biochemistry*, **1989**, 28, 140):

$$v = V_m A / [K_a (1 + I / K_{i, app}) + A] \quad (1)$$

where v is the velocity of the reaction with maximal velocity V_m , A is the concentration of substrate with Michaelis constant of K_a , and I is the concentration of inhibitor.

For those compounds whose progress curves showed downward curvature characteristic of time-dependent inhibition, the data from individual sets was analyzed to give k_{obs} according to equation 2:

$$[AMC] = v_{ss} t + (v_0 - v_{ss}) [1 - \exp(-k_{obs} t)] / k_{obs} \quad (2)$$

where $[AMC]$ is the concentration of product formed over time t , v_0 is the initial reaction velocity and v_{ss} is the final steady state rate. Values for k_{obs} were then analyzed as a linear function of inhibitor concentration to generate an apparent second order rate constant ($k_{obs} / \text{inhibitor concentration}$ or $k_{obs} / [I]$) describing the time-dependent inhibition. A complete discussion of this kinetic treatment has been fully described (Morrison *et al.*, *Adv. Enzymol. Relat. Areas Mol. Biol.*, **1988**, 61, 201).

This assay measures the affinity of inhibitors to cathepsin K. One skilled in the art would consider any compound exhibiting a K_i value of less than 50 micromolar to be a potential lead compound for further research. Preferably, the compounds used in the method of the present invention have a K_i value of less than 1 micromolar. Most preferably, said compounds have a K_i value of less than 100 nanomolar.

Human Osteoclast Resorption Assay

Aliquots of osteoclastoma-derived cell suspensions were removed from liquid nitrogen storage, warmed rapidly at 37°C and washed x1 in RPMI-1640 medium by centrifugation (1000 rpm, 5 min at 4°C). The medium was aspirated and replaced with murine anti-HLA-DR antibody, diluted 1:3 in RPMI-1640 medium, and incubated for 30 min on ice. The cell suspension was mixed frequently.

The cells were washed x2 with cold RPMI-1640 by centrifugation (1000 rpm, 5 min at 4°C) and then transferred to a sterile 15 mL centrifuge tube. The number of mononuclear cells were enumerated in an improved Neubauer counting chamber.

Sufficient magnetic beads (5 / mononuclear cell), coated with goat anti-mouse IgG, were removed from their stock bottle and placed into 5 mL of fresh medium (this washes away the toxic azide preservative). The medium was removed by immobilizing the beads on a magnet and is replaced with fresh medium.

The beads were mixed with the cells and the suspension was incubated for 30 min on ice. The suspension was mixed frequently. The bead-coated cells were immobilized on a magnet and the remaining cells (osteoclast-rich fraction) were decanted into a sterile 50 mL centrifuge tube. Fresh medium was added to the bead-coated cells to dislodge any trapped osteoclasts. This wash process was repeated x10. The bead-coated cells were discarded.

The osteoclasts were enumerated in a counting chamber, using a large-bore disposable plastic Pasteur pipette to charge the chamber with the sample. The cells were pelleted by centrifugation and the density of osteoclasts adjusted to 1.5×10^4 /mL in EMEM medium, supplemented with 10% fetal calf serum and 1.7g/liter of sodium bicarbonate. 3 mL aliquots of the cell suspension (per treatment) were decanted into 15 mL centrifuge tubes. These cells were pelleted by centrifugation. To each tube 3 mL of the appropriate treatment was added (diluted to 50 uM in the EMEM medium). Also included were appropriate vehicle controls, a

positive control (87MEM1 diluted to 100 ug/mL) and an isotype control (IgG2a diluted to 100 ug/mL). The tubes were incubate at 37°C for 30 min.

0.5 mL aliquots of the cells were seeded onto sterile dentine slices in a 48-well plate and incubated at 37°C for 2 h. Each treatment was screened in
5 quadruplicate. The slices were washed in six changes of warm PBS (10 mL / well in a 6-well plate) and then placed into fresh treatment or control and incubated at 37°C for 48 h. The slices were then washed in phosphate buffered saline and fixed in 2% glutaraldehyde (in 0.2M sodium cacodylate) for 5 min., following which they were washed in water and incubated in buffer for 5 min at 37°C. The slices were then
10 washed in cold water and incubated in cold acetate buffer / fast red garnet for 5 min at 4°C. Excess buffer was aspirated, and the slices were air dried following a wash in water.

The TRAP positive osteoclasts were enumerated by bright-field microscopy and were then removed from the surface of the dentine by sonication. Pit volumes
15 were determined using the Nikon/Lasertec ILM21W confocal microscope.

EXAMPLE 3: Method of Detecting Inhibitors

The three dimensional atomic structure can be readily used as a template for selecting potent inhibitors. Various computer programs and databases are available
20 for the purpose. A good inhibitor should at least have excellent steric and electrostatic complementarity to the target, a fair amount of hydrophobic surface buried and sufficient conformational rigidity to minimize entropy loss upon binding. The approach usually comprises several steps:

1) Define a region to target. the active site cavity of cathepsin K can be
25 selected, but any place that is essential to the protease activity could become a potential target. Since the crystal structure has been determined, the spatial and chemical properties of the target region is known.

2) Docking a small molecule onto the target. Many methods can be used to archive this. Computer databases of three-dimensional structures are
30 available for screening millions of small molecular compounds. A negative image of these compounds can be calculated and used to match the shape of the target cavity. The profiles of hydrogen bond donor-acceptor and lipophilic points of these compounds can also be used to complement those of the target. Anyone skilled in the art would be able to identify many small molecules or fragments as hits.

- 3) Linking and extending recognition fragments. Using the hits identified by above procedure, one can incorporate different functional groups or small molecules into a single, larger molecule. The resulting molecule is likely to be more potent and have higher specificity. It is also possible to try to improve the "seed" inhibitor by adding more atoms or fragments that will interact with the target protein. The originally defined target region can be readily expanded to allow further necessary extension.

A limited number of promising compounds can be selected through the process. They can then be synthesized and assayed for their inhibitory properties. The success rate can sometimes be as high as 20%, and it may still be higher with the rapid progresses in computing methods.

EXAMPLE 4: Crystallization of Enzyme with Inhibitors

15 A. Preparation of Inhibitors

Compound 1. Preparation of 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

- 20 a) 3-hydroxy-4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidinecarboxylic acid 1,1dimethylethyl ester

To a solution of 3-hydroxy-4-amino-1-pyrrolidinecarboxylic acid, 1,1-dimethylethyl ester (202 mg, 1.14 mmol) in CH₂Cl₂ (5 mL) was added CBZ-leucine (302.9 mg, 1.14 mmol), HOBT (154 mg, 1.14 mmol) and EDC (262.2 mg, 1.37 mmol). The reaction was allowed to stir until complete by TLC analysis whereupon it was diluted with EtOAc and washed sequentially with pH 4 buffer, sat. K₂CO₃, water and brine. The organic layer was dried (MgSO₄), filtered and concentrated. Column chromatography of the residue (3:1 EtOAc:hexanes) gave 325 mg of the title compound: MS (ES+) 450.3 (MH+), 472.2 (M+Na).

30

- b) 3-hydroxy-4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidine hydrochloride

To a solution of the carbamate (310 mg, 0.69 mmol) in dry EtOAc (5.0 mL) was bubbled HCl gas for approximately 5 minutes. The reaction was stirred until TLC analysis indicated the complete consumption of the starting material. The

35

reaction was then concentrated *in vacuo* to give 249 mg of the title compound: MS (ES+) 350.3 (MH+)

- c) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-
5 [(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinol

To a solution of the amine hydrochloride from the previous step (249 mg, 0.64 mmol) in CH₂Cl₂ (10 mL) was added CBZ-leucine (170.4 mg, 0.64 mmol), HOBT (86.5 mg, 0.64 mmol), NMM (300 μ L) and EDC (147.2 mg, 0.77 mmol). The reaction was allowed to stir at room temperature for 2 hours whereupon it was
10 diluted with ethyl acetate and worked up as described previously. Column chromatography of the residue (3:1 EtOAc:hexanes) gave 104 mg of the title compound: MS (ES+) 597.1 (MH+), 619.1 (M+Na).

- d) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-
15 [(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

To a 0°C solution of the alcohol (100 mg, 0.17 mmol) in acetone (5.0 mL) was added Jones' reagent dropwise until the brown color persisted. The reaction was allowed to warm to room temperature and stirred approximately 48 hours whereupon it was quenched with isopropanol, diluted with EtOAc and washed sequentially with
20 sat. K₂CO₃, water and brine. The organic layer was dried (MgSO₄), filtered and concentrated. Column chromatography of the residue (3:1 EtOAc:hexanes) gave 31 mg of the title compound: MS (ES+) 595.1 (MH+), 617.0 (M+Na).

Compound 2. Preparation of 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-
25 [(methyl)-L-leucyl]-3-pyrrolidinone

- a) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(tert-butoxy)carbonyl]-N-
(methyl)-L-leucyl]-3-pyrrolidinol

To a solution of 3-hydroxy-4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-
30 pyrrolidine (350 mg) was added N-BOC-N-methyl-leucine (222 mg, 0.091 mmol), HOBT (122.5 mg, 0.91 mmol), EDC (208.6 mg, 1.08 mmol) and N-methyl morpholine (0.3 mL, 2.72 mmol). The reaction was stirred at room temperature until complete by TLC analysis. Workup and column chromatography (1:1 Hex:EtOAc) gave 480 mg of the title compound which was used in the following
35 reaction: MS (ES+) 477.4, 577.4 (MH+), 599.4 (M+Na).

b) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(tert-butoxy)carbonyl]-N-(methyl)-L-leucyl]-3-pyrrolidinone

To a -78°C solution of oxalyl chloride (0.11 mL, 1.23 mmol) in CH₂Cl₂ was added DMSO (0.17 mL, 2.46 mmol) dropwise. The reaction was allowed to stir at -78°C for 20 minutes whereupon a solution of the alcohol (474 mg, 0.82 mmol) in CH₂Cl₂ was added dropwise. The reaction was stirred at -78°C for 30 minutes whereupon triethylamine (0.57 mL) was added in a single portion and allowed to warm to room temperature. Workup and column chromatography (2:1 hexanes:ethyl acetate) gave 247 mg of the title compound: MS (ES+) 475, 575 (M+H), 597 (M+Na).

c) 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-L-leucyl]-3-pyrrolidinone hydrochloride

To a room temperature solution EtOAc/HCl was added the carbamate. The reaction was stirred until complete by TLC analysis. Concentration gave the title compound: MS (ES+) 475 (M+H, 100%).

Compound 3. Preparation of 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

a) 3-hydroxy-4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidinecarboxylic acid 1,1-dimethylethyl ester

3-hydroxy-4-amino-1-pyrrolidinecarboxylic acid, 1,1-dimethylethyl ester was coupled with iso-nicotinoyloxycarbonyl leucine in a similar manner as that described above to give 8.5 grams of the title compound: MS (ES+) 451 (MH+, 100%).

b) 3-hydroxy-4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-pyrrolidine hydrochloride

The carbamate from the previous step was deprotected with EtOAc/HCl to give 8.4 grams of the title compound after concentration: MS (ES+) 351 (MH+, 100%).

c) 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinol

To a solution of CBZ leucinal (155 mg) in CH_2Cl_2 was added triethylamine (0.09 mL) and the amine hydrochloride (200 mg, 0.52 mmol) from the previous step. The reaction was stirred at room temperature for 2 hours whereupon the majority of the solvent was removed *in vacuo*. The mixture was redissolved in CH_2Cl_2 and sodium triacetoxyborohydride was added. The reaction was stirred at room temperature for 4 hours. Workup and column chromatography (5% methanol/chloroform) gave 200.5 mg of the title compound: MS(ES+) 583 (MH+, 100%).

- 10 d) 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone
To a DMSO (2 mL) solution of the alcohol (50 mg, 0.09 mmol) from the previous step was added triethylamine (0.07 mL, 0.52 mmol) and pyridine/sulfur trioxide complex (41 mg, 0.26 mmol). The reaction was maintained at room temperature until complete by TLC analysis. Workup and chromatography (5% methanol/chloroform) gave 37 mg of the title compound: MS (ES+) 582 (MH+, 100%).

20 Compound 4. Preparation of (3S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-1-(1-propoxy)-5-methyl-2-hexanone

(3S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-1-diazo-5-methyl-2-hexanone (150 mg, 0.37 mmol) was dissolved in 1-propanol (2.5 ml), then rhodium acetate (2 mg) was added and the reaction was stirred at RT for 2h. The reaction mixture was chromatographed (silica gel, 20% EtOAc/hexanes) to yield the title compound as a white solid (59 mg, 37%). MS(ES) $\text{M}+\text{H}^+ = 435$, $\text{M}+\text{NH}_4^+ = 452$, $2\text{M}+\text{H}^+ = 869.6$.

30 Compound 5. Preparation of bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one

Cbz-leucine (500 mg, 1.88 mmol), EDCI (558 mg, 1.88 mmol) was dissolved in DMF (4.0 ml) with 1,3-diamino-propan-2-ol (85 mg, 0.94 mmol) and Hunig's base (0.3 ml, 1.88 mmol) and was stirred at RT overnight. The reaction was diluted with EtOAc (20 ml) and was extracted with water (2 x 20 ml). The combined organics were dried with magnesium sulfate, filtered, concentrated in vacuo. The intermediate was then dissolved in acetone (4.0 ml) and Jones reagent

(2.0 ml, 1.5 M) was added dropwise and the reaction was stirred at RT overnight. The excess Jones reagent was then quenched with isopropanol (1.0 ml), then the reaction was diluted with EtOAc (20 ml) and was extracted with water (2x 20 ml) to remove the inorganic salts. The combined organics were dried with magnesium sulfate, filtered, concentrated, and chromatographed (silica gel, 2-5% MeOH/methylene chloride) to give the title compound as a white solid (410 mg, 75%).
MS(ES) $M+H^+=583$, $M+Na^+=605$.

10 Compound 6. Preparation of 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leuciny)]carbohydrazide

a) methyl 3-benzyloxybenzoate

To a suspension of NaH (0.395 g, 9.87 mmol, 60% in mineral oil) in DMF (20 mL) was added methyl 3-hydroxybenzoate (1.0 g, 6.58 mmol). After stirring for 15 min at room temperature, benzyl bromide (1.1 g, 6.58 mmol) was added. After stirring at room temperature for 3h, the solution was partitioned between ethyl acetate and water. The organic layer was washed with water (2 X 75 mL), saturated aqueous sodium bicarbonate, and brine, then dried ($MgSO_4$), filtered and concentrated to yield an off-white solid (1.013 g, 4.2 mmol). 1H NMR (400 MHz, $CDCl_3$) δ 7.67 (m, 2H), 7.48-7.34 (m, 6H), 7.19 (m, 1H), 5.12 (s, 2H), 3.95 (s, 3H).

b) 3-benzyloxybenzoic acid

To a solution of the compound of Example 6(a) (0.400 g, 1.65 mmol) in THF (2 mL) and water (2 mL) was added lithium hydroxide monohydrate (0.076 g, 1.82 mmol). After stirring at reflux for 5 h, the solution was partitioned between ethyl acetate and 3N HCl. The organic layer was washed with brine, dried ($MgSO_4$), filtered and concentrated to yield a white solid (0.355 g, 1.56 mmol). 1H NMR (400 MHz, CD_3OD) δ 7.58 (m, 2H), 7.36-7.24 (m, 6H), 7.10 (m, 1H), 5.04 (s, 2H).

30 c) 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leuciny)]carbohydrazide

Following the procedure of Example A, below, except substituting 3-benzyloxybenzoic acid for N-acetyl-L-leucine and 2-[N-(N-benzyloxycarbonyl-L-leuciny)]carbohydrazide for 2-[N-(N-benzyloxycarbonyl-L-alany)]carbohydrazide,

the title compound was prepared as a white solid (0.062 g, 25%). MS(ESI): 548.1 (M+H)⁺.

Example A

5 Preparation of 2-[N-(N-acetyl-L-leuciny)]-2'-[N'-(N-benzyloxycarbonyl-L-alanyl)]carbohydrazide

To a stirring solution of 2-[N-(N-benzyloxycarbonyl-L-alanyl)]carbohydrazide (0.150g, 0.508mmol) in DMF (2mL) was added N-acetyl-L-leucine (0.092g, 0.534mmol), 1-hydroxybenzotriazole (0.014g, 0.102mmol), and 1-
 10 (3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (0.102g, 0.534mmol). After stirring at room temperature for 16h, the solution was diluted with ethyl acetate, washed successively with water, saturated aqueous sodium bicarbonate, and brine. The organic layer was dried (MgSO₄), filtered and concentrated. The residue was purified by column chromatography (silica gel, methanol/dichloromethane) to
 15 yield the title compound as a white solid (0.028 g, 12%). MS(ESI): 451.1 (M+H)⁺.

Compound 7. Preparation of (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leuciny)hydrazide

20 a) N-*tert*-butoxycarbonyl-(L)-leucinamide

To a solution of N-*tert*-butoxycarbonyl-(L)-leucine (7.0g, 28.1mmol) in dry THF (100mL) at -40°C was added isobutylchloroformate (3.8g, 28.1mmol) and N-methylmorpholine (6.0, 59mmol). After 15 minutes of stirring, ammonia was bubbled through the mixture for an additional 15 minutes, then warmed to room
 25 temperature and allowed to stir for 2 hours. Mixture filtered and filtrate concentrated in vacuo to yield title compound as a white solid (6.5, 28.0mmol). ¹HNMR (400MHz, CDCl₃) δ 6.38 (br s, 1H), 5.79 (br s, 1H), 5.04 (br d, 1H), 4.13 (m, 1H), 1.71-1.49 (m, 3H), 1.39 (s, 9H), 0.92 (dd, 6H).

30 b) N-*tert*-butoxycarbonyl-(L)-leucine thioamide

To a stirring solution of the compound of Example 7(a) (6.5, 28.0 mmol) in dry THF was added Lawesson's reagent (6.8g, 16.9 mmol) and the mixture was stirred at room temperature under argon overnight. The solvent was evaporated and the residue chromatographed (silica gel, 12% ethyl acetate/hexane) to give the title
 35 compound as a white solid (5.4g, 77%). ¹HNMR (400MHz, CDCl₃) δ 8.54 (br s,

1H), 7.97 (br s, 1H), 5.28 (br d, 1H), 4.52 (m, 1H), 1.72-1.58 (m, 3H), 1.40 (s, 9H), 0.92 (m, 6H).

c) (1S)-1-(tert-butoxycarbonyl)amino-1-(4-carboethoxythiazol-2-yl)-3-methylbutane

The compound of Example 7(b) (5.4g, 21.7 mmol) was stirred in dry acetone (100mL) under argon at -10°C. Ethylbromopyruvate (4.7g, 23.9mmol) was added and stirred for 1h at -10°C. The solution was poured into a well stirred mixture of chloroform and water and then into saturated sodium bicarbonate solution. The organic phase was separated and the aqueous layer extracted with chloroform. The combined organic extracts were dried over MgSO₄, filtered and concentrated to an oil. The oily residue was treated with TFAA (5.0g, 23.9mmol) and pyridine (3.8g, 47.8mmol) in dichloromethane for 1h at -20°C. Excess solvent was removed in vacuo and the residue was dissolved in dichloromethane. The solution was washed with saturated aqueous sodium bicarbonate and 1.0N KHSO₄ until pH 7. The solution was dried over magnesium sulfate, filtered and concentrated to an oil which was chromatographed (silica gel, 7.5% ethyl acetate/hexane) to give the title compound as a tan solid (4.5g, 61%). ¹HNMR (400MHz, CDCl₃) δ 7.98 (s, 1H), 5.04 (br d, 1H), 4.95 (m, 1H), 4.31 (q, 2H), 1.88 (m, 1H), 1.63 (m, 2H), 1.40 (s, 9H), 1.32 (t, 3H), 0.85 (dd, 6H).

d) (1S)-1-(Benzyloxycarbonyl)amino-1-(4-carboethoxythiazol-2-yl)-3-methylbutane

The compound of Example 7(c) (0.250g, 0.731mmol) was dissolved in TFA (2mL) and stirred at room temperature for 15 minutes when diluted with methanol and concentrated in vacuo. The residue was dissolved in methylene chloride and treated with triethylamine (0.739g, 7.31mmol) followed by benzyl chloroformate (1.2g, 7.31mmol). The solution stirred at room temperature for 2h when partition between ethyl acetate/water. The organic layer was washed with brine, collected, dried (MgSO₄) and concentrated to a residue that was chromatographed (silica gel, 15% ethyl acetate/hexane) to give the title compound as an oil (0.198g, 72%). ¹HNMR (400MHz, CDCl₃) δ 8.01 (s, 1H), 7.32 (m, 5H), 5.51 (br d, 1H), 5.14 (m, 1H), 5.10 (s, 2H), 4.37 (q, 2H), 1.93 (m, 1H), 1.81-1.67 (m, 2H), 1.39 (t, 3H), 0.95 (m, 6H).

e) (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leuciny)hydrazide

Following the procedure of Example B(a)-(d), below, except substituting
5 (1S)-1-(Benzyloxycarbonyl)amino-1-(4-carboethoxythiazol-2-yl)-3-methylbutane
for (1S)-1-benzyloxycarbonylamino-1-(2-carboethoxythiazol-4-yl)-3-methylbutane
in step (c), the title compound was prepared. MS (MH⁺): 610.0

Example B

10 Preparation of (1S,2'R)-N-4-[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-2-ylcarbonyl-N'-2'-(benzyloxycarbonyl)amino-4'-methylpentanoylhydrazide

a) N-benzyloxycarbonyl-L-leuciny bromomethyl ketone

1-methyl-3-nitro-1-nitrosoguanidine (6.65 g, 45.2 mmol) in ether (225 mL)
15 is cooled to 0°C. 40% sodium hydroxide is added slowly and the diazomethane is
allowed to collect in the ether solution for 30 minutes at 0°C. The ether solution is
then decanted and left at 0 °C.

N-Cbz-L-leucine (2.10 g, 7.6 mmol) was dissolved in THF (10 mL), cooled
to -40 °C, and 4-methylmorpholine (0.77 g, 7.6 mmol, 0.83 mL) was added,
20 followed by dropwise addition of isobutyl chloroformate (1.04 g, 7.6 mmol, 0.98
mL). After 15 min, the solution was filtered into the previously prepared 0 °C
solution of ethereal diazomethane. The resulting solution was allowed to stand at 0
°C for 23 h. HBr (30% in acetic acid) (45.2 mmol, 9 mL) was added and the
resulting solution was stirred at 0 °C for 5 min, then washed sequentially with 0.1 N
25 HCl, saturated aqueous NaHCO₃ and saturated brine, then dried (MgSO₄), filtered
and concentrated to give the title compound as a colorless oil (2.43 g, 94%).

b) (1S)-1-benzyloxycarbonylamino-1-(2-carboethoxythiazol-4-yl)-3-methylbutane

A solution of the compound of Example B(a) (1.57 g, 4.58 mmol) and ethyl
30 thiooxamate (0.61 g, 4.58 mmol) in ethanol (10 mL) was heated at reflux for 4 h.
The solution was then cooled, concentrated and the residue was purified by flash
chromatography on 230-400 mesh silica gel, eluting with 1:4 ethyl acetate/hexanes,
to give the title compound as a yellow oil (1.0 g, 58%). ¹H NMR (400 MHz,
CDCl₃) δ 7.41 (s, 1H), 7.34-7.31 (m, 5H), 5.40 (d, 1H), 5.10 (d, 1H), 5.05 (d, 1H),

4.98 (q, 1H), 4.48 (q, 2H), 1.80-1.76 (m, 2H), 1.57-1.53 (m, 1H), 1.44 (t, 3H), 0.95 (d, 3H), 0.93 (d, 3H).

5 c) (1S)-1-benzyloxycarbonylamino-1-(2-hydrazinocarbonylthiazol-4-yl)-3-methylbutane

A solution of the compound of Example B(b) (0.30 g, 0.8 mmol) and hydrazine hydrate (0.40 g, 8.0 mmol, 0.39 mL) in ethanol (8 mL) was allowed to stir at room temperature for 2 h. The solution was then concentrated to yield the title compound as a white foam (0.28 g, 98%). ¹H NMR (400 MHz, CDCl₃) δ 8.29 (s, 1H), 7.37-7.35 (m, 5H), 5.18 (d, 1H), 5.09 (dd, 2H), 4.95 (q, 1H), 4.07 (d, 2H), 1.71 (t, 2H), 1.55 (m, 1H), 0.96 (d, 3H), 0.94 (d, 3H).

15 d) (1S,2'R)-N-4-[[[(1-benzyloxycarbonyl)amino]-3-methylbutyl]thiazol-2-yl]carbonyl-N'-2'-(benzyloxycarbonyl)amino-4'-methylpentanoylhydrazide

A solution of the compound of Example B(c) (100 mg, 0.28 mmol), N-Cbz-L-leucine (80.5 mg, 0.30 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (58.2 mg, 0.30 mmol) and 1-hydroxybenzotriazole (7.5 mg, 0.06 mmol) in DMF (0.6 mmol) was allowed to stir at room temperature for 18 h. The solution was diluted with ethyl acetate and washed successively with water, 0.1 N HCl, saturated aqueous NaHCO₃ and saturated brine, then dried (MgSO₄), filtered and concentrated. The residue was purified by flash chromatography on 230-400 mesh silica gel, eluting with 1:1 ethyl acetate/hexanes, to provide the title compound as a white solid (111.4 mg, 66%). mp 110-112 °C.

Compound 8. Preparation of 2,2'-N,N'-bis-benzylloxycarbonyl-L-leucinylcarbohydrazide

To a stirring solution of N-Cbz-L-leucine (Chemical Dynamics Corp.) (2.94 g, 11.1 mmol) in 22 mL of DMF was added carbohydrazide (0.5 g, 5.6 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (2.13 g, 11.1 mmol) and 1-hydroxybenzotriazole (0.3 g, 2.2 mmol). After stirring at room temperature for 22 h, the solution was poured into 500 mL of water. The precipitate was collected by vacuum filtration and washed with water (4 X 150 mL) and dichloromethane (4 X 150 mL), then dried under vacuum to provide the title compound as a white solid (1.49 g, 46%). MS(ESI): 607.1 (M+Na)⁺.

Compound 9. Preparation of 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one

a) 1-N-(N-imidazole acetyl-leucinyl)-amino-3-N-(4-phenoxy phenyl sulfonyl)-amino-propan-2-one

Following the procedure of Example C(a)-(d), below, substituting "imidazole acetic acid" for "4-pyridyl acetic acid", the title compound was prepared: MS(ES) M +H⁺ = 542.

Example C

Preparation of 1-N-(N-Cbz-leucinyl)-amino-3-N-(2-pyridyl-sulfonyl)-amino-propan-2-one

a) 1-N-(N-Cbz-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-ol

1,3-Diamino propan-2-ol (6.75 g, 75 mmol) was dissolved in DMF (100ml) and Cbz-leucine (20g, 75.5 mmol), HOBt-hydrate (11g, 81.5 mmol), and EDCI (15.5g, 81.2 mmol) were added. The reaction was stirred overnight at RT. A portion of the reaction mixture (30 ml) was concentrated in vacuo, then ether (50 ml) and MeOH (30 ml) were added. A 1N solution of hydrochloric acid in ether was added (1 M, 30 ml) and a white gum formed, which was washed several times with ether. MeOH-acetone were added and heated until the gum became a white solid.

The white solid was dissolved in DMF (25 ml) and DIEA (5ml), then 4-phenoxy

phenyl sulfonyl chloride was added. The reaction was stirred for 2h, concentrated in vacuo, then chromatographed (silica gel, 1:1 EtOAc: hexanes) to provide the desired product as a white solid.

- 5 b) Leucinyl-amino-3-N-(4-phenoxy phenyl sulfonyl)-amino-propan-2-ol
 1-N-(Cbz-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-
 2-ol (1.0g, 1.8 mmol) was dissolved in EtOH (30 ml), then 10% Pd/C (0.22g) was
 added followed by 6N hydrochloric acid (2.5 ml), and the reaction was stirred under
 a balloon of hydrogen gas for 4h at RT. The reaction mixture was filtered,
10 concentrated, and azeotroped with toluene to provide a white glass which was used
 in the next reaction without further purification.
- c) 1-N-(N-4-pyridyl acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-
 amino-propan-2-ol
15 Leucinyl-amino-3-N-(4-phenoxy phenyl sulfonyl)-amino-propan-2-ol (0.36
 g, 0.76 mmol) was dissolved in DMF (5 ml), then NMM (0.45 ml, 4 mmol) was
 added followed by 4-pyridyl acetic acid (0.13g, 0.75 mmol) and HBTU (0.29g, 0.76
 mmol) and the reaction was stirred at RT overnight. The reaction mixture was
 concentrated in vacuo, then chromatographed (silica gel, 5%MeOH: methylene
20 chloride) to provide the desired product as a white solid (90 mg, MS(ES): $M+H^+ =$
 555.
- d) 1-N-(N-4-pyridyl acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-
 amino-propan-2-one
25 1-N-(N-4-pyridyl-acetyl-leucinyl)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-
 amino-propan-2-ol (45 mg, 0.08 mmol) was dissolved in acetone (5ml), then 1N
 hydrochloric acid (2 ml) was added. The reaction was concentrated in vacuo, then
 redissolved in acetone. Jones reagent (1.5 M, several drops) was added and the
 reaction mixture was stirred for 6h at RT. Isopropanol (0.5 ml) was added and the
30 reaction mixture was concentrated in vacuo. The reaction was diluted with pH 7
 buffer and then was extracted with EtOAc, dried with magnesium sulfate, filtered,
 concentrated in vacuo, then chromatographed (silica gel, 5% MeOH-methylene
 chloride) to give the desired product as a white solid (27 mg, 50%): MS(ES):
 $M+H^+ = 553$.

35

B. Crystallization of the protein and protein-inhibitor complexes

Human cathepsin K was expressed in *baculovirus* cells for the first eight of the nine inhibitors described below. Conditioned media containing expressed pro-cathepsin K was loaded directly onto an S-Sepharose column pre-equilibrated with 25 mM phosphate buffer at pH 8. The column was eluted with a NaCl gradient. Fractions containing pro-cathepsin K were pooled, concentrated to 2.5 mg/ml and activated to mature cathepsin K in 50 mM sodium acetate buffer pH 4.0 containing 20 mM L-cysteine and 1% mature cathepsin K as seed. The activation was monitored using CBZ-Phe-Arg-AMC, as fluorogenic substrate and by SDS-PAGE. When the increasing specific activity reached a plateau (*ca.* 15 μ mol/min/mg), the reaction was stopped by the addition of inhibitor. The inhibited mature cathepsin K was concentrated and dialyzed against 20 mM MES, 50 mM NaCl, 2 mM L-cysteine, pH 6.

Protein preparation for cathepsin K complex with 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[(N-(methyl)-L-leucyl)]-3-pyrrolidinone (only)

Human cathepsin K was expressed in *E. coli*. The cell pellet from 1 L of bacterial culture weighing 2.35 gm. was washed with 50 mL of 50 mM Tris/HCl, 5 mM EDTA, 150 mM NaCl, pH 8.0. After centrifugation at 13,000 x g for 15 mins, the washed pellet was resuspended into 25 mL of the same buffer prepared at 4° C and lysed by passage twice through a cell disruptor (Avestin) at 10,000 psi. The lysate was centrifuged as above, the supernatant decanted and the pellet suspended in 25 mL 50 mM Tris/HCl, 10 mM DTT, 5 mM EDTA, 150 mM NaCl, pH 8.0 containing either 8 M urea or 6 M guanidine HCl. After stirring at 4° C for 30 mins, insoluble cellular debris was removed by centrifugation at 23,000 x g for 30 mins and the supernatant clarified by filtration (0.45 μ m, Millipore).

Varying amounts of the proenzyme form of cathepsin K were refolded by quick dilution into stirring, N₂ (g) sparged 50 mM Tris/HCl, 5 mM EDTA, 10 mM reduced and 1 mM oxidized glutathione, 0.7 M L-arginine pH 8.0 and stirred overnight at 4° C. After concentration to *ca.* 1 mg/mL using a stirred cell fitted with a YM-10 membrane (Amicon), the sample was clarified by centrifugation and filtration then dialyzed against 25 mM Na₂PO₄, 1.0 M NaCl, pH 7.0. The dialysate was applied at a LFR= 23 cm/hr to

a 2.6 x 90 cm column of Superdex 75 (Pharmacia) pre-equilibrated in 25 mM Na₂PO₄, 1.0 M NaCl, pH 7.0. The cathepsin K proenzyme was pooled based upon purity as observed on a reduced, SDS-PAGE gel.

5 Crystals of mature activated cathepsin K complexed with inhibitor grew to a size of approximately 0.2 mm³ in about six days at 20°C. The concentration of inhibited cathepsin K used in the crystallization was approximately 8 mg./ml. The method of vapor diffusion in hanging drops was used to grow crystals from the solution of cathepsin K - inhibitor complex. The initial crystal structure to be
10 determined was that of cathepsin K in complex with the cysteine protease inhibitor E64. Crystals of mature activated cathepsin K complexed with E-64 grew to a size of approximately 0.2 mm³ in six days at 20°C. The concentration of E-64-inhibited cathepsin K used in the crystallization was 8 mg/ml. Vapor diffusion was used in hanging drops from a solution of 10% PEG 8000, 0.1 M Na⁺/K⁺ phosphate at pH
15 6.2 containing 0.2M NaCl. Crystals of the complex are orthorhombic, space group P2₁2₁2₁, with cell constants of a=38.4, b=50.7, and c=104.9 Ångstroms. This crystal form will be referred to as Form II. The crystals contain one molecule in the asymmetric unit and contain approximately 40% solvent with a V_m value of 2.1 Å³/Dalton. X-ray diffraction data were measured from a single crystal using a
20 Siemens two-dimensional position-sensitive detector on a Siemens rotating anode generate operating a 5 KW. The structure was determined by molecular replacement using X-PLOR. The starting model consisted of all atoms of the main chain of papain and those side chain atoms predicted to be homologous between the two proteins as determined from sequence alignment. The cross rotation function was
25 calculated using x-ray diffraction data from 10 to 4 Å and a radius of integration of 32 Å. The highest peak was 6.0 σ. A translation search was carried out using data from 8 to 3.5 Ångstroms resulting in the highest peak of 12.5 σ. The resulting model gave an R_c factor of 0.488. This model was refined by rigid-body refinement, and the resulting phases were used to calculate Fourier maps with coefficients |F_O-F_C|
30 and |2F_O-F_C|, into which the atomic model of cathepsin K was built using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. The structure was refined using X-PLOR. The electron density for E-64 was clear in the maps. The inhibitor was built into density and several additional cycles of map fitting and refinement were carried
35 out to a final R_c of 0.191.

Crystallization of the complex of cathepsin K with 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone

- 5 Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 10% isopropanol, 0.1 M NaPO₄ / citrate at pH 4.2. Crystals of the complex are tetragonal, space group P4₃2₁2, with cell constants of a=57.6 Å, and c=131.2 Å. This crystal form will be referred to as Form III. Diffraction data were collected as described above. The crystals contain one molecule in the asymmetric
- 10 unit and contain 36% solvent with a V_m value of 2.3 Å³/Dalton. The structure was determined by molecular replacement using X-PLOR at 2.5 Ångstroms resolution. The starting model consisted of all protein atoms of the orthorhombic form of cathepsin K-E64 structure. Molecular replacement was carried out as described above for the cathepsin K-E64 structure determination. The model was refined by
- 15 rigid-body refinement using X-PLOR, and the resulting phases were used to calculate Fourier maps with coefficients |F_o-F_c| and |2F_o-F_c|, into which the atomic model of the inhibitor was built using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. The structure was refined using X-PLOR. Several cycles of map fitting and
- 20 refinement were carried out to a final R_c of 0.245.

Crystallization of the complex of cathepsin K with 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl)-L-leucinyl]carbohydrazide

- 25 Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 22.5% PEG 8000, 0.075 M sodium acetate at pH 4.5 containing 0.15 M Li₂SO₄. Crystals of the complex grew as Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement with X-PLOR utilizing the previous Form III protein model at 2.4 Ångstroms resolution.
- 30 Fourier maps with coefficients |F_o-F_c| and |2F_o-F_c| were used to fit the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement (X-PLOR) was used to refine the structure during model building. Several cycles of map fitting and refinement were carried out to a final R_c of 0.237.

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Crystallization of the complex of cathepsin K with bis-(Cbz-leucinyl)-1,3-diamino-propan-2-one

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 10% isopropanol, 0.1 M NaPO₄ / citrate at pH 4.2. Crystals of the complex grow as Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form III protein model at 2.6 Ångstroms resolution. Fourier maps with coefficients $|F_O - F_C|$ and $|2F_O - F_C|$ were used to fit the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. Several cycles of map fitting and refinement were carried out using X-PLOR to a final R_C of 0.210.

Crystallization of the complex of cathepsin K with 4-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[(methyl)-L-leucyl]-3-pyrrolidinone

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution 18% PEG 8000, 0.6 M sodium acetate at pH 4.5 containing 0.12 M Li₂SO₄. Crystals of the complex grow in Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form III protein model with X-PLOR at 2.4 Ångstroms resolution. Fourier maps with coefficients $|F_O - F_C|$ and $|2F_O - F_C|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_C of 0.218.

Crystallization of the complex of cathepsin K with (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-yl]carbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyl)hydrazide

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 30% MPD, 0.1 M MES at pH 7.0 and 0.1 M tris buffer at pH 7.0. Crystals of the complex are Form II. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.3 Ångstroms resolution. Fourier maps with

coefficients $|F_o - F_c|$ and $|2F_o - F_c|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.211.

5

Crystallization of the complex of cathepsin K with 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 33% MPD, 0.1 M MES at pH 7. Crystals of the complex grow as Form II. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.2 Ångstroms resolution. Fourier maps with coefficients $|F_o - F_c|$ and $|2F_o - F_c|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.208.

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Crystallization of the complex of cathepsin K with 4-[N-

[(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

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Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 28% MPD, 0.1 M MES at pH 7.0 and 0.1 M tris buffer at pH 7.0.

Crystals of the complex Form II. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.3 Ångstroms resolution. Fourier maps with coefficients $|F_o - F_c|$ and $|2F_o - F_c|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several cycles of map fitting and refinement were carried out to a final R_c of 0.193.

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Crystallization of the complex of cathepsin K with 4-[N-[(4-

pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone

35

Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 30% MPD, 0.1 M MES at pH 7.0 and 0.1 M tris buffer at pH 7.0.

Crystals of the complex Form II. Diffraction data were collected as described above.

- 5 The structure was determined by rigid body refinement of the previous Form II protein model with X-PLOR at 2.2 Å resolution. Fourier maps with coefficients $|F_O - F_C|$ and $|2F_O - F_C|$, were used to the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building using X-PLOR. Several
10 cycles of map fitting and refinement were carried out to a final R_C of 0.267.

Crystallization of the complex of cathepsin K with 1-N-(N-imidazole acetyl-leuciny)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one

- 15 Crystals of mature activated cathepsin K complexed with the inhibitor grew from a solution of 18% PEG 8000, 0.6 M sodium acetate at pH 4.5 containing 0.12 M Li_2SO_4 . Crystals of the complex are Form III. Diffraction data were collected as described above. The structure was determined by rigid body refinement of the previous Form II protein model at 2.5 Å resolution. Fourier maps with
20 coefficients $|F_O - F_C|$ and $|2F_O - F_C|$ were used to fit the atomic model of the inhibitor using the molecular graphics program FRODO. Conventional positional refinement was used to refine the structure during model building. Several cycles of map fitting and refinement were carried out using X-PLOR to a final R_C of 0.246.

Abbreviations

- 25 E-64, [1-[N-[(L-3-*trans*-carboxyoxirane-2-carbonyl)-L-leucyl]amino]-4-guanidinobutane]
CBZ, benzyloxycarbonyl
AMC, aminomethylcoumarin
30 MPD, 2-methyl-2,4-pentanediol
PIPES, piperazine-N,N-bis(2-ethanesulfonic acid)
MES, 2-(N-morpholino)-ethanesulfonic acid
tris, tris(hydroxymethyl)-aminomethane
PEG, polyethyleneglycol
35 M, Molar

$$R_c = \Sigma(F_o - F_c) / F_o$$

F_o = observed structure amplitude

F_c = calculated structure amplitude

EDTA, ethylenediaminetetraacetic acid

5 DTT, 1,4-dithiothreitol

SDS-PAGE, sodium dodecylsulfate polyacrylamide gel electrophoresis

This invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those
10 described herein will become apparent to those skilled in the art from the foregoing description. Such modifications are intended to fall within the scope of the appended claims.

The disclosures of the patents, patent applications and publications cited herein are incorporated by reference in their entireties.

TABLE I

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for cathepsin K.

Residue Atom	X	Y	Z	B
1 ALA N	-3.94	11.01	90.45	15.00
1 ALA CA	-4.70	12.30	90.45	15.00
1 ALA C	-4.40	13.14	89.20	15.00
1 ALA O	-3.34	12.99	88.57	15.00
1 ALA CB	-4.36	13.12	91.73	15.00
2 PRO N	-5.36	14.01	88.80	15.00
2 PRO CA	-5.19	14.86	87.61	15.00
2 PRO C	-4.35	16.05	88.06	15.00
2 PRO O	-4.89	17.00	88.65	15.00
2 PRO CB	-6.62	15.33	87.31	15.00
2 PRO CG	-7.53	14.58	88.32	15.00
2 PRO CD	-6.63	14.31	89.47	15.00
3 ASP N	-3.04	16.00	87.87	15.00
3 ASP CA	-2.25	17.14	88.30	15.00
3 ASP C	-2.27	18.18	87.20	15.00
3 ASP O	-1.57	18.02	86.20	15.00
3 ASP CB	-0.82	16.75	88.67	15.00
3 ASP CG	-0.09	17.85	89.45	15.00
3 ASP OD1	-0.74	18.83	89.89	15.00
3 ASP OD2	1.14	17.73	89.63	15.00
4 SER N	-3.10	19.21	87.36	15.00
4 SER CA	-3.19	20.26	86.35	15.00
4 SER C	-3.97	21.51	86.77	15.00
4 SER O	-4.97	21.44	87.48	15.00
4 SER CB	-3.77	19.72	85.03	15.00
4 SER OG	-5.17	19.55	85.08	15.00
5 VAL N	-3.50	22.65	86.28	15.00
5 VAL CA	-4.10	23.94	86.54	15.00
5 VAL C	-4.27	24.65	85.17	15.00
5 VAL O	-3.43	24.48	84.28	15.00
5 VAL CB	-3.22	24.79	87.51	15.00
5 VAL CG1	-1.80	24.88	87.00	15.00
5 VAL CG2	-3.79	26.17	87.69	15.00
6 ASP N	-5.39	25.34	84.99	15.00
6 ASP CA	-5.67	26.08	83.76	15.00
6 ASP C	-6.40	27.34	84.22	15.00
6 ASP O	-7.63	27.33	84.43	15.00
6 ASP CB	-6.55	25.25	82.82	15.00
6 ASP CG	-6.81	25.95	81.48	15.00

TABLE I

6 ASP OD1	-6.11	26.94	81.14	15.00
6 ASP OD2	-7.72	25.49	80.75	15.00
7 TYR N	-5.64	28.42	84.37	15.00
7 TYR CA	-6.15	29.70	84.84	15.00
7 TYR C	-7.18	30.35	83.96	15.00
7 TYR O	-7.76	31.36	84.33	15.00
7 TYR CB	-5.00	30.67	85.09	15.00
7 TYR CG	-4.06	30.20	86.18	15.00
7 TYR CD1	-4.41	30.29	87.52	15.00
7 TYR CD2	-2.82	29.64	85.86	15.00
7 TYR CE1	-3.55	29.86	88.52	15.00
7 TYR CE2	-1.96	29.21	86.84	15.00
7 TYR CZ	-2.33	29.31	88.17	15.00
7 TYR OH	-1.48	28.86	89.14	15.00
8 ARG N	-7.41	29.78	82.79	15.00
8 ARG CA	-8.41	30.30	81.87	15.00
8 ARG C	-9.77	30.07	82.53	15.00
8 ARG O	-10.65	30.93	82.49	15.00
8 ARG CB	-8.33	29.58	80.53	15.00
8 ARG CG	-7.00	29.76	79.85	15.00
8 ARG CD	-7.00	29.12	78.48	15.00
8 ARG NE	-7.27	27.69	78.52	15.00
8 ARG CZ	-6.85	26.83	77.58	15.00
8 ARG NH1	-6.15	27.27	76.54	15.00
8 ARG NH2	-7.15	25.54	77.69	15.00
9 LYS N	-9.90	28.94	83.20	15.00
9 LYS CA	-11.12	28.60	83.91	15.00
9 LYS C	-11.16	29.33	85.28	15.00
9 LYS O	-11.96	28.99	86.15	15.00
9 LYS CB	-11.18	27.08	84.13	15.00
9 LYS CG	-11.04	26.25	82.86	15.00
9 LYS CD	-11.09	24.72	83.11	15.00
9 LYS CE	-9.80	24.15	83.76	15.00
9 LYS NZ	-9.78	22.65	83.99	15.00
10 LYS N	-10.33	30.35	85.47	15.00
10 LYS CA	-10.28	31.03	86.76	15.00
10 LYS C	-10.23	32.55	86.69	15.00
10 LYS O	-10.11	33.20	87.73	15.00
10 LYS CB	-9.10	30.51	87.58	15.00
10 LYS CG	-9.05	28.98	87.72	15.00
10 LYS CD	-7.68	28.45	88.13	15.00
10 LYS CE	-7.54	28.31	89.63	15.00
10 LYS NZ	-7.61	29.62	90.36	15.00
11 GLY N	-10.29	33.11	85.48	15.00

TABLE I

11	GLY	CA	-10.27	34.56	85.31	15.00
11	GLY	C	-8.96	35.28	85.53	15.00
11	GLY	O	-8.93	36.49	85.77	15.00
12	TYR	N	-7.86	34.54	85.44	15.00
12	TYR	CA	-6.54	35.11	85.64	15.00
12	TYR	C	-5.97	35.67	84.36	15.00
12	TYR	O	-5.13	36.58	84.39	15.00
12	TYR	CB	-5.57	34.04	86.13	15.00
12	TYR	CG	-5.76	33.63	87.56	15.00
12	TYR	CD1	-6.85	32.86	87.95	15.00
12	TYR	CD2	-4.82	33.98	88.52	15.00
12	TYR	CE1	-7.00	32.46	89.25	15.00
12	TYR	CE2	-4.96	33.58	89.83	15.00
12	TYR	CZ	-6.04	32.81	90.19	15.00
12	TYR	OH	-6.16	32.38	91.49	15.00
13	VAL	N	-6.40	35.09	83.24	15.00
13	VAL	CA	-5.92	35.47	81.92	15.00
13	VAL	C	-6.95	36.24	81.09	15.00
13	VAL	O	-8.15	36.03	81.21	15.00
13	VAL	CB	-5.41	34.21	81.15	15.00
13	VAL	CG1	-6.54	33.26	80.89	15.00
13	VAL	CG2	-4.73	34.61	79.86	15.00
14	THR	N	-6.45	37.19	80.31	15.00
14	THR	CA	-7.27	38.02	79.44	15.00
14	THR	C	-7.39	37.38	78.05	15.00
14	THR	O	-6.69	36.41	77.74	15.00
14	THR	CB	-6.63	39.42	79.32	15.00
14	THR	OG1	-5.21	39.28	79.27	15.00
14	THR	CG2	-7.00	40.28	80.52	15.00
15	PRO	N	-8.31	37.88	77.20	15.00
15	PRO	CA	-8.50	37.34	75.86	15.00
15	PRO	C	-7.23	37.45	75.01	15.00
15	PRO	O	-6.38	38.30	75.30	15.00
15	PRO	CB	-9.61	38.22	75.30	15.00
15	PRO	CG	-10.38	38.60	76.51	15.00
15	PRO	CD	-9.28	38.96	77.45	15.00
16	VAL	N	-7.14	36.65	73.95	15.00
16	VAL	CA	-5.97	36.64	73.08	15.00
16	VAL	C	-5.86	37.87	72.18	15.00
16	VAL	O	-6.80	38.23	71.47	15.00
16	VAL	CB	-5.94	35.38	72.22	15.00
16	VAL	CG1	-4.70	35.38	71.34	15.00
16	VAL	CG2	-5.97	34.18	73.10	15.00
17	LYS	N	-4.70	38.52	72.22	15.00

TABLE I

17 LYS CA	-4.47	39.71	71.43	15.00
17 LYS C	-3.49	39.39	70.31	15.00
17 LYS O	-2.82	38.36	70.34	15.00
17 LYS CB	-3.93	40.85	72.30	15.00
17 LYS CG	-4.99	41.75	72.95	15.00
17 LYS CD	-5.84	41.01	73.99	15.00
17 LYS CE	-5.88	41.72	75.34	15.00
17 LYS NZ	-4.53	41.86	75.97	15.00
18 ASN N	-3.43	40.30	69.35	15.00
18 ASN CA	-2.58	40.20	68.17	15.00
18 ASN C	-1.54	41.29	68.24	15.00
18 ASN O	-1.89	42.46	68.35	15.00
18 ASN CB	-3.42	40.41	66.91	15.00
18 ASN CG	-2.71	39.96	65.64	15.00
18 ASN OD1	-1.74	40.58	65.19	15.00
18 ASN ND2	-3.19	38.87	65.06	15.00
19 GLN N	-0.27	40.92	68.15	15.00
19 GLN CA	0.79	41.91	68.23	15.00
19 GLN C	0.97	42.67	66.95	15.00
19 GLN O	1.54	43.76	66.94	15.00
19 GLN CB	2.10	41.26	68.59	15.00
19 GLN CG	2.54	40.22	67.63	15.00
19 GLN CD	3.88	39.71	67.99	15.00
19 GLN OE1	4.04	38.93	68.92	15.00
19 GLN NE2	4.89	40.20	67.31	15.00
20 GLY N	0.51	42.07	65.86	15.00
20 GLY CA	0.62	42.69	64.56	15.00
20 GLY C	1.98	42.49	63.90	15.00
20 GLY O	2.53	41.39	63.86	15.00
21 GLN N	2.50	43.60	63.38	15.00
21 GLN CA	3.77	43.62	62.67	15.00
21 GLN C	4.94	43.82	63.62	15.00
21 GLN O	6.05	43.35	63.36	15.00
21 GLN CB	3.73	44.74	61.64	15.00
21 GLN CG	2.68	44.55	60.56	15.00
21 GLN CD	2.88	43.25	59.82	15.00
21 GLN OE1	4.01	42.87	59.52	15.00
21 GLN NE2	1.79	42.55	59.56	15.00
22 CYS N	4.68	44.56	64.69	15.00
22 CYS CA	5.65	44.87	65.73	15.00
22 CYS C	6.15	43.60	66.46	15.00
22 CYS O	5.37	42.68	66.72	15.00
22 CYS CB	4.97	45.82	66.71	15.00
22 CYS SG	5.96	46.40	68.11	15.00

TABLE I

23	GLY N	7.45	43.53	66.73	15.00
23	GLY CA	8.00	42.37	67.42	15.00
23	GLY C	7.84	42.62	68.90	15.00
23	GLY O	8.80	42.94	69.61	15.00
24	SER N	6.60	42.54	69.37	15.00
24	SER CA	6.33	42.80	70.77	15.00
24	SER C	5.75	41.63	71.54	15.00
24	SER O	4.72	41.77	72.20	15.00
24	SER CB	5.44	44.05	70.90	15.00
24	SER OG	4.14	43.81	70.40	15.00
25	CYC N	6.39	40.47	71.48	15.00
25	CYC CA	5.88	39.34	72.25	15.00
25	CYC CB	6.32	38.03	71.63	15.00
25	CYC SG	8.04	38.06	71.17	15.00
25	CYC C	6.33	39.44	73.72	15.00
25	CYC O	5.67	38.91	74.62	15.00
25	CYC O1	7.96	38.09	69.44	15.00
26	TRP N	7.45	40.14	73.95	15.00
26	TRP CA	7.97	40.33	75.30	15.00
26	TRP C	7.04	41.24	76.05	15.00
26	TRP O	6.67	40.96	77.18	15.00
26	TRP CB	9.37	40.92	75.27	15.00
26	TRP CG	9.47	42.24	74.61	15.00
26	TRP CD1	9.74	42.49	73.30	15.00
26	TRP CD2	9.32	43.52	75.24	15.00
26	TRP NE1	9.78	43.84	73.06	15.00
26	TRP CE2	9.52	44.50	74.24	15.00
26	TRP CE3	9.04	43.94	76.55	15.00
26	TRP CZ2	9.45	45.88	74.51	15.00
26	TRP CZ3	8.98	45.32	76.82	15.00
26	TRP CH2	9.18	46.27	75.80	15.00
27	ALA N	6.63	42.32	75.39	15.00
27	ALA CA	5.70	43.30	75.95	15.00
27	ALA C	4.40	42.61	76.34	15.00
27	ALA O	3.92	42.75	77.47	15.00
27	ALA CB	5.43	44.39	74.93	15.00
28	PHE N	3.83	41.86	75.40	15.00
28	PHE CA	2.60	41.13	75.63	15.00
28	PHE C	2.79	40.08	76.73	15.00
28	PHE O	2.00	40.02	77.66	15.00
28	PHE CB	2.10	40.48	74.33	15.00
28	PHE CG	1.41	41.44	73.39	15.00
28	PHE CD1	2.14	42.29	72.57	15.00
28	PHE CD2	0.02	41.51	73.33	15.00

TABLE I

28 PHE CE1	1.51	43.18	71.73	15.00
28 PHE CE2	-0.62	42.40	72.49	15.00
28 PHE CZ	0.12	43.24	71.69	15.00
29 SER N	3.85	39.28	76.64	15.00
29 SER CA	4.15	38.25	77.64	15.00
29 SER C	4.33	38.84	79.03	15.00
29 SER O	3.95	38.23	80.03	15.00
29 SER CB	5.43	37.50	77.25	15.00
29 SER OG	5.78	36.51	78.20	15.00
30 SER N	4.96	40.01	79.08	15.00
30 SER CA	5.18	40.71	80.33	15.00
30 SER C	3.84	41.16	80.89	15.00
30 SER O	3.48	40.84	82.03	15.00
30 SER CB	6.10	41.91	80.10	15.00
30 SER OG	7.39	41.48	79.72	15.00
31 VAL N	3.08	41.87	80.07	15.00
31 VAL CA	1.75	42.34	80.48	15.00
31 VAL C	0.85	41.18	80.88	15.00
31 VAL O	0.03	41.31	81.77	15.00
31 VAL CB	1.09	43.16	79.36	15.00
31 VAL CG1	-0.41	43.10	79.47	15.00
31 VAL CG2	1.57	44.60	79.43	15.00
32 GLY N	1.05	40.04	80.24	15.00
32 GLY CA	0.26	38.85	80.51	15.00
32 GLY C	0.56	38.20	81.83	15.00
32 GLY O	-0.24	37.41	82.32	15.00
33 ALA N	1.74	38.46	82.39	15.00
33 ALA CA	2.10	37.90	83.69	15.00
33 ALA C	1.61	38.88	84.75	15.00
33 ALA O	1.01	38.49	85.75	15.00
33 ALA CB	3.59	37.68	83.80	15.00
34 LEU N	1.79	40.17	84.49	15.00
34 LEU CA	1.35	41.21	85.40	15.00
34 LEU C	-0.15	41.08	85.64	15.00
34 LEU O	-0.65	41.47	86.69	15.00
34 LEU CB	1.64	42.59	84.83	15.00
34 LEU CG	3.09	42.99	84.57	15.00
34 LEU CD1	3.08	44.29	83.81	15.00
34 LEU CD2	3.84	43.15	85.87	15.00
35 GLU N	-0.88	40.56	84.67	15.00
35 GLU CA	-2.32	40.39	84.82	15.00
35 GLU C	-2.66	39.14	85.64	15.00
35 GLU O	-3.66	39.11	86.37	15.00
35 GLU CB	-2.98	40.28	83.45	15.00

TABLE I

35	GLU	CG	-2.84	41.50	82.57	15.00
35	GLU	CD	-3.34	41.23	81.17	15.00
35	GLU	OE1	-3.19	40.08	80.70	15.00
35	GLU	OE2	-3.87	42.16	80.54	15.00
36	GLY	N	-1.84	38.10	85.50	15.00
36	GLY	CA	-2.08	36.89	86.26	15.00
36	GLY	C	-1.99	37.16	87.76	15.00
36	GLY	O	-2.78	36.62	88.55	15.00
37	GLN	N	-1.03	37.99	88.17	15.00
37	GLN	CA	-0.86	38.31	89.57	15.00
37	GLN	C	-1.88	39.32	90.06	15.00
37	GLN	O	-2.40	39.18	91.17	15.00
37	GLN	CB	0.55	38.83	89.86	15.00
37	GLN	CG	1.61	37.74	90.00	15.00
37	GLN	CD	1.14	36.57	90.83	15.00
37	GLN	OE1	0.97	36.67	92.05	15.00
37	GLN	NE2	0.93	35.43	90.17	15.00
38	LEU	N	-2.17	40.32	89.23	15.00
38	LEU	CA	-3.14	41.34	89.61	15.00
38	LEU	C	-4.49	40.73	90.02	15.00
38	LEU	O	-5.12	41.20	90.95	15.00
38	LEU	CB	-3.34	42.35	88.48	15.00
38	LEU	CG	-4.22	43.54	88.86	15.00
38	LEU	CD1	-3.64	44.20	90.08	15.00
38	LEU	CD2	-4.33	44.53	87.71	15.00
39	LYS	N	-4.92	39.70	89.30	15.00
39	LYS	CA	-6.18	39.02	89.60	15.00
39	LYS	C	-6.00	38.22	90.90	15.00
39	LYS	O	-6.92	38.19	91.73	15.00
39	LYS	CB	-6.58	38.09	88.45	15.00
39	LYS	CG	-7.57	36.99	88.79	15.00
39	LYS	CD	-8.95	37.51	89.13	15.00
39	LYS	CE	-9.89	36.35	89.41	15.00
39	LYS	NZ	-11.25	36.77	89.82	15.00
40	LYS	N	-4.83	37.60	91.07	15.00
40	LYS	CA	-4.57	36.82	92.28	15.00
40	LYS	C	-4.64	37.74	93.49	15.00
40	LYS	O	-5.25	37.40	94.51	15.00
40	LYS	CB	-3.20	36.16	92.21	15.00
40	LYS	CG	-3.09	34.85	92.98	15.00
40	LYS	CD	-1.63	34.41	93.04	15.00
40	LYS	CE	-1.44	33.15	93.86	15.00
40	LYS	NZ	0.00	32.80	94.08	15.00
41	LYS	N	-4.06	38.93	93.36	15.00

TABLE I

41	LYS	CA	-4.06	39.93	94.43	15.00
41	LYS	C	-5.40	40.66	94.59	15.00
41	LYS	O	-6.17	40.38	95.49	15.00
41	LYS	CB	-2.93	40.95	94.23	15.00
41	LYS	CG	-1.55	40.33	94.11	15.00
41	LYS	CD	-1.34	39.26	95.18	15.00
41	LYS	CE	-0.06	38.46	94.95	15.00
41	LYS	NZ	-0.04	37.19	95.74	15.00
42	THR	N	-5.69	41.58	93.67	15.00
42	THR	CA	-6.91	42.36	93.75	15.00
42	THR	C	-8.23	41.65	93.40	15.00
42	THR	O	-9.28	42.28	93.37	15.00
42	THR	CB	-6.77	43.64	92.91	15.00
42	THR	OG1	-6.89	43.34	91.51	15.00
42	THR	CG2	-5.40	44.26	93.16	15.00
43	GLY	N	-8.17	40.35	93.10	15.00
43	GLY	CA	-9.38	39.62	92.78	15.00
43	GLY	C	-10.09	39.89	91.44	15.00
43	GLY	O	-10.94	39.09	91.03	15.00
44	LYS	N	-9.82	41.02	90.79	15.00
44	LYS	CA	-10.45	41.31	89.50	15.00
44	LYS	C	-9.41	41.72	88.45	15.00
44	LYS	O	-8.48	42.49	88.73	15.00
44	LYS	CB	-11.57	42.34	89.64	15.00
44	LYS	CG	-11.20	43.55	90.45	15.00
44	LYS	CD	-12.43	44.28	90.95	15.00
44	LYS	CE	-12.02	45.39	91.93	15.00
44	LYS	NZ	-11.26	44.88	93.11	15.00
45	LEU	N	-9.60	41.19	87.25	15.00
45	LEU	CA	-8.69	41.41	86.13	15.00
45	LEU	C	-8.92	42.66	85.26	15.00
45	LEU	O	-10.04	43.15	85.12	15.00
45	LEU	CB	-8.71	40.16	85.25	15.00
45	LEU	CG	-7.54	39.90	84.33	15.00
45	LEU	CD1	-6.25	39.87	85.12	15.00
45	LEU	CD2	-7.75	38.59	83.63	15.00
46	LEU	N	-7.83	43.15	84.69	15.00
46	LEU	CA	-7.84	44.31	83.80	15.00
46	LEU	C	-6.81	44.09	82.69	15.00
46	LEU	O	-5.76	43.51	82.93	15.00
46	LEU	CB	-7.44	45.58	84.55	15.00
46	LEU	CG	-8.49	46.47	85.20	15.00
46	LEU	CD1	-7.96	47.90	85.21	15.00
46	LEU	CD2	-9.77	46.43	84.42	15.00

TABLE I

47 ASN N	-7.11	44.56	81.49	15.00
47 ASN CA	-6.17	44.43	80.38	15.00
47 ASN C	-5.12	45.50	80.56	15.00
47 ASN O	-5.45	46.67	80.62	15.00
47 ASN CB	-6.88	44.66	79.03	15.00
47 ASN CG	-7.67	43.45	78.57	15.00
47 ASN OD1	-7.13	42.37	78.38	15.00
47 ASN ND2	-8.97	43.65	78.34	15.00
48 LEU N	-3.86	45.10	80.70	15.00
48 LEU CA	-2.77	46.07	80.88	15.00
48 LEU C	-2.15	46.34	79.52	15.00
48 LEU O	-2.28	45.53	78.61	15.00
48 LEU CB	-1.74	45.56	81.90	15.00
48 LEU CG	-2.26	45.06	83.27	15.00
48 LEU CD1	-1.09	44.75	84.18	15.00
48 LEU CD2	-3.18	46.08	83.91	15.00
49 SER N	-1.46	47.47	79.36	15.00
49 SER CA	-0.91	47.82	78.06	15.00
49 SER C	0.51	47.42	77.67	15.00
49 SER O	1.48	47.79	78.33	15.00
49 SER CB	-1.10	49.32	77.77	15.00
49 SER OG	-0.19	50.13	78.51	15.00
50 PRO N	0.64	46.66	76.56	15.00
50 PRO CA	1.94	46.22	76.04	15.00
50 PRO C	2.59	47.44	75.41	15.00
50 PRO O	3.80	47.52	75.25	15.00
50 PRO CB	1.54	45.21	74.97	15.00
50 PRO CG	0.21	44.71	75.44	15.00
50 PRO CD	-0.45	45.98	75.85	15.00
51 GLN N	1.74	48.40	75.03	15.00
51 GLN CA	2.18	49.65	74.43	15.00
51 GLN C	3.01	50.45	75.42	15.00
51 GLN O	4.12	50.87	75.11	15.00
51 GLN CB	0.97	50.49	74.00	15.00
51 GLN CG	1.33	51.66	73.08	15.00
51 GLN CD	1.77	51.20	71.71	15.00
51 GLN OE1	0.96	50.74	70.92	15.00
51 GLN NE2	3.06	51.26	71.44	15.00
52 ASN N	2.47	50.66	76.62	15.00
52 ASN CA	3.18	51.42	77.65	15.00
52 ASN C	4.59	50.85	77.83	15.00
52 ASN O	5.56	51.59	77.97	15.00
52 ASN CB	2.42	51.35	78.97	15.00
52 ASN CG	3.09	52.12	80.09	15.00

TABLE I

52	ASN	OD1	2.74	51.95	81.25	15.00
52	ASN	ND2	4.04	52.99	79.74	15.00
53	LEU	N	4.68	49.53	77.81	15.00
53	LEU	CA	5.95	48.86	77.94	15.00
53	LEU	C	6.82	49.21	76.72	15.00
53	LEU	O	7.87	49.84	76.88	15.00
53	LEU	CB	5.75	47.35	78.08	15.00
53	LEU	CG	5.11	46.95	79.41	15.00
53	LEU	CD1	4.91	45.45	79.49	15.00
53	LEU	CD2	6.00	47.41	80.54	15.00
54	VAL	N	6.33	48.87	75.52	15.00
54	VAL	CA	7.03	49.15	74.25	15.00
54	VAL	C	7.63	50.55	74.20	15.00
54	VAL	O	8.85	50.72	74.04	15.00
54	VAL	CB	6.06	49.01	73.03	15.00
54	VAL	CG1	6.70	49.55	71.75	15.00
54	VAL	CG2	5.67	47.56	72.83	15.00
55	ASP	N	6.76	51.55	74.37	15.00
55	ASP	CA	7.12	52.96	74.31	15.00
55	ASP	C	8.05	53.45	75.40	15.00
55	ASP	O	8.84	54.37	75.19	15.00
55	ASP	CB	5.85	53.84	74.36	15.00
55	ASP	CG	4.87	53.56	73.22	15.00
55	ASP	OD1	5.23	52.86	72.24	15.00
55	ASP	OD2	3.72	54.05	73.29	15.00
56	CYS	N	7.97	52.82	76.56	15.00
56	CYS	CA	8.76	53.27	77.70	15.00
56	CYS	C	9.97	52.47	78.16	15.00
56	CYS	O	10.98	53.06	78.54	15.00
56	CYS	CB	7.81	53.52	78.84	15.00
56	CYS	SG	6.36	54.45	78.28	15.00
57	VAL	N	9.87	51.15	78.17	15.00
57	VAL	CA	10.98	50.31	78.60	15.00
57	VAL	C	12.16	50.44	77.62	15.00
57	VAL	O	12.50	49.50	76.90	15.00
57	VAL	CB	10.54	48.83	78.71	15.00
57	VAL	CG1	11.66	47.98	79.32	15.00
57	VAL	CG2	9.26	48.72	79.52	15.00
58	SER	N	12.85	51.57	77.67	15.00
58	SER	CA	13.98	51.87	76.80	15.00
58	SER	C	15.15	50.91	76.84	15.00
58	SER	O	16.13	51.10	76.13	15.00
58	SER	CB	14.48	53.27	77.09	15.00
58	SER	OG	14.95	53.34	78.42	15.00

TABLE I

59	GLU N	15.09	49.92	77.71	15.00
59	GLU CA	16.15	48.93	77.82	15.00
59	GLU C	15.93	47.86	76.73	15.00
59	GLU O	16.77	46.99	76.50	15.00
59	GLU CB	16.14	48.30	79.22	15.00
59	GLU CG	16.39	49.27	80.39	15.00
59	GLU CD	15.13	49.97	80.88	15.00
59	GLU OE1	14.38	49.38	81.70	15.00
59	GLU OE2	14.90	51.13	80.46	15.00
60	ASN N	14.77	47.91	76.10	15.00
60	ASN CA	14.43	46.98	75.04	15.00
60	ASN C	14.26	47.73	73.71	15.00
60	ASN O	13.99	48.94	73.69	15.00
60	ASN CB	13.13	46.26	75.38	15.00
60	ASN CG	13.27	45.35	76.57	15.00
60	ASN OD1	12.35	45.22	77.38	15.00
60	ASN ND2	14.41	44.68	76.68	15.00
61	ASP N	14.39	47.02	72.61	15.00
61	ASP CA	14.25	47.65	71.31	15.00
61	ASP C	12.82	48.03	70.94	15.00
61	ASP O	12.60	48.65	69.91	15.00
61	ASP CB	14.84	46.75	70.23	15.00
61	ASP CG	15.93	47.43	69.44	15.00
61	ASP OD1	15.87	48.66	69.28	15.00
61	ASP OD2	16.85	46.72	68.98	15.00
62	GLY N	11.84	47.67	71.77	15.00
62	GLY CA	10.46	47.99	71.45	15.00
62	GLY C	9.91	47.03	70.41	15.00
62	GLY O	9.71	45.85	70.70	15.00
63	CYS N	9.68	47.50	69.20	15.00
63	CYS CA	9.19	46.60	68.16	15.00
63	CYS C	10.33	45.71	67.70	15.00
63	CYS O	10.09	44.70	67.04	15.00
63	CYS CB	8.59	47.36	66.99	15.00
63	CYS SG	6.94	48.02	67.38	15.00
64	GLY N	11.56	46.10	68.03	15.00
64	GLY CA	12.72	45.32	67.68	15.00
64	GLY C	12.90	44.16	68.64	15.00
64	GLY O	13.65	43.21	68.37	15.00
65	GLY N	12.20	44.23	69.78	15.00
65	GLY CA	12.28	43.17	70.77	15.00
65	GLY C	12.86	43.58	72.11	15.00
65	GLY O	13.34	44.70	72.31	15.00
66	GLY N	12.81	42.65	73.05	15.00

TABLE I

66 GLY CA	13.34	42.92	74.37	15.00
66 GLY C	13.08	41.77	75.32	15.00
66 GLY O	12.42	40.80	74.94	15.00
67 TYR N	13.57	41.90	76.55	15.00
67 TYR CA	13.40	40.87	77.56	15.00
67 TYR C	12.23	41.18	78.48	15.00
67 TYR O	11.93	42.34	78.75	15.00
67 TYR CB	14.68	40.76	78.39	15.00
67 TYR CG	15.91	40.56	77.55	15.00
67 TYR CD1	16.20	39.32	76.98	15.00
67 TYR CD2	16.77	41.61	77.29	15.00
67 TYR CE1	17.33	39.13	76.18	15.00
67 TYR CE2	17.90	41.44	76.49	15.00
67 TYR CZ	18.18	40.20	75.94	15.00
67 TYR OH	19.27	40.05	75.12	15.00
68 MET N	11.57	40.13	78.99	15.00
68 MET CA	10.45	40.33	79.90	15.00
68 MET C	10.90	40.92	81.23	15.00
68 MET O	10.21	41.72	81.83	15.00
68 MET CB	9.72	39.00	80.18	15.00
68 MET CG	8.97	38.38	79.00	15.00
68 MET SD	9.97	37.36	77.92	15.00
68 MET CE	11.01	36.45	79.11	15.00
69 THR N	12.09	40.53	81.68	15.00
69 THR CA	12.62	41.03	82.94	15.00
69 THR C	12.76	42.55	82.93	15.00
69 THR O	12.33	43.21	83.87	15.00
69 THR CB	13.98	40.37	83.29	15.00
69 THR OG1	14.96	40.72	82.30	15.00
69 THR CG2	13.84	38.85	83.35	15.00
70 ASN N	13.33	43.09	81.85	15.00
70 ASN CA	13.53	44.54	81.73	15.00
70 ASN C	12.24	45.34	81.80	15.00
70 ASN O	12.25	46.51	82.16	15.00
70 ASN CB	14.28	44.87	80.45	15.00
70 ASN CG	15.72	44.45	80.52	15.00
70 ASN OD1	16.11	43.68	81.39	15.00
70 ASN ND2	16.54	44.97	79.61	15.00
71 ALA N	11.14	44.68	81.45	15.00
71 ALA CA	9.81	45.28	81.50	15.00
71 ALA C	9.27	45.18	82.93	15.00
71 ALA O	8.72	46.14	83.46	15.00
71 ALA CB	8.88	44.57	80.51	15.00
72 PHE N	9.46	44.02	83.55	15.00

TABLE I

72 PHE CA	9.02	43.79	84.93	15.00
72 PHE C	9.63	44.86	85.81	15.00
72 PHE O	8.94	45.51	86.59	15.00
72 PHE CB	9.49	42.43	85.44	15.00
72 PHE CG	8.73	41.28	84.88	15.00
72 PHE CD1	7.40	41.42	84.52	15.00
72 PHE CD2	9.34	40.04	84.73	15.00
72 PHE CE1	6.67	40.35	84.03	15.00
72 PHE CE2	8.62	38.96	84.24	15.00
72 PHE CZ	7.29	39.12	83.89	15.00
73 GLN N	10.93	45.05	85.64	15.00
73 GLN CA	11.67	46.04	86.41	15.00
73 GLN C	11.17	47.48	86.11	15.00
73 GLN O	11.29	48.37	86.94	15.00
73 GLN CB	13.16	45.86	86.13	15.00
73 GLN CG	14.11	46.75	86.94	15.00
73 GLN CD	14.52	46.20	88.32	15.00
73 GLN OE1	15.45	46.73	88.93	15.00
73 GLN NE2	13.85	45.16	88.80	15.00
74 TYR N	10.54	47.68	84.96	15.00
74 TYR CA	10.04	49.00	84.58	15.00
74 TYR C	8.81	49.41	85.38	15.00
74 TYR O	8.69	50.56	85.81	15.00
74 TYR CB	9.72	49.05	83.08	15.00
74 TYR CG	8.90	50.26	82.67	15.00
74 TYR CD1	9.48	51.52	82.60	15.00
74 TYR CD2	7.54	50.14	82.44	15.00
74 TYR CE1	8.71	52.63	82.31	15.00
74 TYR CE2	6.77	51.25	82.15	15.00
74 TYR CZ	7.36	52.49	82.09	15.00
74 TYR OH	6.58	53.59	81.84	15.00
75 VAL N	7.87	48.48	85.54	15.00
75 VAL CA	6.65	48.74	86.31	15.00
75 VAL C	7.07	49.05	87.76	15.00
75 VAL O	6.41	49.80	88.47	15.00
75 VAL CB	5.73	47.48	86.38	15.00
75 VAL CG1	4.32	47.87	86.73	15.00
75 VAL CG2	5.77	46.72	85.07	15.00
76 GLN N	8.18	48.44	88.18	15.00
76 GLN CA	8.71	48.62	89.52	15.00
76 GLN C	9.26	50.02	89.71	15.00
76 GLN O	8.62	50.86	90.31	15.00
76 GLN CB	9.78	47.57	89.79	15.00
76 GLN CG	10.35	47.60	91.20	15.00

TABLE I

76 GLN CD	11.53	46.64	91.36	15.00
76 GLN OE1	12.17	46.25	90.38	15.00
76 GLN NE2	11.80	46.25	92.59	15.00
77 LYS N	10.43	50.30	89.15	15.00
77 LYS CA	11.04	51.62	89.32	15.00
77 LYS C	10.24	52.83	88.85	15.00
77 LYS O	10.34	53.90	89.44	15.00
77 LYS CB	12.44	51.64	88.71	15.00
77 LYS CG	12.52	51.06	87.30	15.00
77 LYS CD	13.96	50.69	86.97	15.00
77 LYS CE	14.06	49.75	85.79	15.00
77 LYS NZ	15.39	49.07	85.82	15.00
78 ASN N	9.48	52.69	87.77	15.00
78 ASN CA	8.67	53.81	87.31	15.00
78 ASN C	7.51	53.96	88.28	15.00
78 ASN O	6.94	55.03	88.41	15.00
78 ASN CB	8.12	53.56	85.90	15.00
78 ASN CG	7.17	54.66	85.44	15.00
78 ASN OD1	7.61	55.76	85.09	15.00
78 ASN ND2	5.88	54.37	85.44	15.00
79 ARG N	7.19	52.86	88.95	15.00
79 ARG CA	6.11	52.78	89.94	15.00
79 ARG C	4.71	52.88	89.33	15.00
79 ARG O	4.05	53.92	89.37	15.00
79 ARG CB	6.31	53.81	91.08	15.00
79 ARG CG	7.67	53.69	91.80	15.00
79 ARG CD	7.80	54.56	93.06	15.00
79 ARG NE	6.84	54.23	94.12	15.00
79 ARG CZ	6.60	53.00	94.59	15.00
79 ARG NH1	7.24	51.94	94.09	15.00
79 ARG NH2	5.73	52.83	95.58	15.00
80 GLY N	4.27	51.76	88.76	15.00
80 GLY CA	2.95	51.68	88.15	15.00
80 GLY C	2.98	51.54	86.64	15.00
80 GLY O	3.87	52.07	85.97	15.00
81 ILE N	1.98	50.85	86.10	15.00
81 ILE CA	1.88	50.64	84.66	15.00
81 ILE C	0.45	50.97	84.23	15.00
81 ILE O	-0.49	50.68	84.96	15.00
81 ILE CB	2.19	49.17	84.30	15.00
81 ILE CG1	2.27	48.99	82.78	15.00
81 ILE CG2	1.14	48.24	84.90	15.00
81 ILE CD1	2.64	47.59	82.36	15.00
82 ASP N	0.29	51.58	83.05	15.00

TABLE I

82 ASP CA	-1.04	51.93	82.56	15.00
82 ASP C	-1.89	50.76	82.07	15.00
82 ASP O	-1.38	49.69	81.71	15.00
82 ASP CB	-0.93	52.93	81.42	15.00
82 ASP CG	-0.47	54.29	81.87	15.00
82 ASP OD1	-0.66	54.63	83.06	15.00
82 ASP OD2	0.08	55.02	81.02	15.00
83 SER N	-3.20	50.96	82.05	15.00
83 SER CA	-4.12	49.95	81.56	15.00
83 SER C	-4.32	50.20	80.07	15.00
83 SER O	-4.22	51.34	79.61	15.00
83 SER CB	-5.46	50.02	82.32	15.00
83 SER OG	-6.06	51.30	82.22	15.00
84 GLU N	-4.61	49.14	79.32	15.00
84 GLU CA	-4.81	49.22	77.86	15.00
84 GLU C	-5.66	50.40	77.38	15.00
84 GLU O	-5.20	51.19	76.57	15.00
84 GLU CB	-5.39	47.91	77.33	15.00
84 GLU CG	-5.73	47.89	75.85	15.00
84 GLU CD	-4.51	47.97	74.94	15.00
84 GLU OE1	-3.51	47.25	75.17	15.00
84 GLU OE2	-4.57	48.74	73.96	15.00
85 ASP N	-6.87	50.53	77.90	15.00
85 ASP CA	-7.72	51.61	77.45	15.00
85 ASP C	-7.12	52.99	77.70	15.00
85 ASP O	-7.49	53.97	77.03	15.00
85 ASP CB	-9.10	51.52	78.07	15.00
85 ASP CG	-10.07	52.52	77.46	15.00
85 ASP OD1	-9.97	52.79	76.24	15.00
85 ASP OD2	-10.93	53.06	78.21	15.00
86 ALA N	-6.18	53.08	78.64	15.00
86 ALA CA	-5.54	54.36	78.93	15.00
86 ALA C	-4.30	54.57	78.04	15.00
86 ALA O	-3.90	55.70	77.78	15.00
86 ALA CB	-5.16	54.45	80.40	15.00
87 TYR N	-3.74	53.48	77.53	15.00
87 TYR CA	-2.56	53.54	76.67	15.00
87 TYR C	-2.69	52.41	75.64	15.00
87 TYR O	-1.98	51.39	75.73	15.00
87 TYR CB	-1.32	53.33	77.55	15.00
87 TYR CG	-0.03	53.89	77.01	15.00
87 TYR CD1	0.20	53.99	75.64	15.00
87 TYR CD2	0.99	54.29	77.89	15.00
87 TYR CE1	1.41	54.47	75.16	15.00

TABLE I

87 TYR CE2	2.20	54.77	77.41	15.00
87 TYR CZ	2.41	54.86	76.05	15.00
87 TYR OH	3.61	55.32	75.57	15.00
88 PRO N	-3.60	52.58	74.65	15.00
88 PRO CA	-3.93	51.66	73.55	15.00
88 PRO C	-2.80	51.22	72.61	15.00
88 PRO O	-2.08	52.05	72.06	15.00
88 PRO CB	-5.01	52.43	72.79	15.00
88 PRO CG	-5.64	53.28	73.84	15.00
88 PRO CD	-4.42	53.80	74.54	15.00
89 TYR N	-2.74	49.92	72.34	15.00
89 TYR CA	-1.71	49.35	71.48	15.00
89 TYR C	-1.83	49.79	70.01	15.00
89 TYR O	-2.46	49.11	69.21	15.00
89 TYR CB	-1.74	47.82	71.56	15.00
89 TYR CG	-0.54	47.18	70.92	15.00
89 TYR CD1	0.75	47.59	71.30	15.00
89 TYR CD2	-0.66	46.24	69.91	15.00
89 TYR CE1	1.88	47.07	70.69	15.00
89 TYR CE2	0.47	45.70	69.28	15.00
89 TYR CZ	1.74	46.13	69.68	15.00
89 TYR OH	2.87	45.65	69.09	15.00
90 VAL N	-1.19	50.88	69.65	15.00
90 VAL CA	-1.22	51.40	68.29	15.00
90 VAL C	-0.55	50.51	67.23	15.00
90 VAL O	-0.83	50.63	66.03	15.00
90 VAL CB	-0.63	52.83	68.21	15.00
90 VAL CG1	-1.26	53.71	69.28	15.00
90 VAL CG2	0.88	52.80	68.33	15.00
91 GLY N	0.37	49.65	67.64	15.00
91 GLY CA	1.01	48.77	66.67	15.00
91 GLY C	2.38	49.17	66.15	15.00
91 GLY O	2.89	48.57	65.20	15.00
92 GLN N	3.00	50.17	66.77	15.00
92 GLN CA	4.32	50.61	66.35	15.00
92 GLN C	4.96	51.34	67.52	15.00
92 GLN O	4.33	51.51	68.57	15.00
92 GLN CB	4.21	51.53	65.13	15.00
92 GLN CG	3.46	52.85	65.38	15.00
92 GLN CD	3.28	53.70	64.12	15.00
92 GLN OE1	3.93	54.73	63.94	15.00
92 GLN NE2	2.39	53.25	63.25	15.00
93 GLU N	6.19	51.79	67.34	15.00
93 GLU CA	6.90	52.49	68.39	15.00

TABLE I

93 GLU C	6.60	53.99	68.38	15.00
93 GLU O	6.84	54.67	67.38	15.00
93 GLU CB	8.41	52.27	68.23	15.00
93 GLU CG	8.80	50.81	68.17	15.00
93 GLU CD	10.30	50.60	68.23	15.00
93 GLU OE1	10.85	50.53	69.35	15.00
93 GLU OE2	10.93	50.50	67.15	15.00
94 GLU N	6.08	54.49	69.49	15.00
94 GLU CA	5.76	55.90	69.63	15.00
94 GLU C	6.54	56.47	70.80	15.00
94 GLU O	7.40	55.80	71.37	15.00
94 GLU CB	4.27	56.10	69.86	15.00
94 GLU CG	3.45	56.13	68.58	15.00
94 GLU CD	1.96	56.28	68.85	15.00
94 GLU OE1	1.48	55.64	69.81	15.00
94 GLU OE2	1.27	57.03	68.11	15.00
95 SER N	6.22	57.71	71.14	15.00
95 SER CA	6.84	58.41	72.26	15.00
95 SER C	6.16	57.91	73.52	15.00
95 SER O	4.92	57.82	73.58	15.00
95 SER CB	6.63	59.93	72.12	15.00
95 SER OG	5.25	60.23	71.89	15.00
96 CYS N	6.96	57.55	74.51	15.00
96 CYS CA	6.44	57.04	75.77	15.00
96 CYS C	5.44	58.02	76.39	15.00
96 CYS O	5.84	59.03	76.95	15.00
96 CYS CB	7.59	56.77	76.74	15.00
96 CYS SG	7.00	56.38	78.40	15.00
97 MET N	4.15	57.73	76.21	15.00
97 MET CA	3.06	58.55	76.74	15.00
97 MET C	2.40	58.00	78.01	15.00
97 MET O	1.16	57.90	78.06	15.00
97 MET CB	1.97	58.73	75.69	15.00
97 MET CG	2.36	59.52	74.45	15.00
97 MET SD	1.29	58.98	73.09	15.00
97 MET CE	-0.36	59.43	73.71	15.00
98 TYR N	3.20	57.65	79.01	15.00
98 TYR CA	2.67	57.13	80.26	15.00
98 TYR C	1.93	58.21	81.06	15.00
98 TYR O	2.48	59.26	81.38	15.00
98 TYR CB	3.78	56.51	81.11	15.00
98 TYR CG	3.32	56.04	82.48	15.00
98 TYR CD1	3.24	56.92	83.56	15.00
98 TYR CD2	2.95	54.72	82.69	15.00

TABLE I

98 TYR CE1	2.81	56.49	84.80	15.00
98 TYR CE2	2.52	54.29	83.95	15.00
98 TYR CZ	2.45	55.18	84.99	15.00
98 TYR OH	2.02	54.77	86.22	15.00
99 ASN N	0.69	57.92	81.43	15.00
99 ASN CA	-0.14	58.84	82.20	15.00
99 ASN C	-0.54	58.20	83.54	15.00
99 ASN O	-1.31	57.23	83.58	15.00
99 ASN CB	-1.37	59.22	81.36	15.00
99 ASN CG	-2.38	60.08	82.13	15.00
99 ASN OD1	-2.01	60.89	82.99	15.00
99 ASN ND2	-3.66	59.90	81.80	15.00
100 PRO N	-0.02	58.74	84.65	15.00
100 PRO CA	-0.30	58.24	86.00	15.00
100 PRO C	-1.77	58.23	86.33	15.00
100 PRO O	-2.22	57.46	87.19	15.00
100 PRO CB	0.45	59.22	86.90	15.00
100 PRO CG	1.58	59.70	86.02	15.00
100 PRO CD	0.86	59.92	84.71	15.00
101 THR N	-2.53	59.08	85.65	15.00
101 THR CA	-3.96	59.13	85.89	15.00
101 THR C	-4.56	57.81	85.43	15.00
101 THR O	-5.64	57.43	85.89	15.00
101 THR CB	-4.63	60.25	85.10	15.00
101 THR OG1	-3.86	61.45	85.21	15.00
101 THR CG2	-6.03	60.52	85.66	15.00
102 GLY N	-3.86	57.13	84.52	15.00
102 GLY CA	-4.33	55.86	84.01	15.00
102 GLY C	-3.55	54.62	84.42	15.00
102 GLY O	-3.52	53.65	83.67	15.00
103 LYS N	-2.90	54.62	85.59	15.00
103 LYS CA	-2.15	53.44	86.02	15.00
103 LYS C	-3.12	52.35	86.50	15.00
103 LYS O	-4.26	52.65	86.86	15.00
103 LYS CB	-1.13	53.83	87.11	15.00
103 LYS CG	-1.51	53.50	88.56	15.00
103 LYS CD	-0.97	52.13	88.98	15.00
103 LYS CE	-1.39	51.77	90.40	15.00
103 LYS NZ	-1.11	50.35	90.75	15.00
104 ALA N	-2.68	51.10	86.52	15.00
104 ALA CA	-3.55	50.01	86.96	15.00
104 ALA C	-2.86	48.86	87.68	15.00
104 ALA O	-3.52	47.92	88.12	15.00
104 ALA CB	-4.37	49.49	85.79	15.00

TABLE I

105 ALA N	-1.55	48.92	87.82	15.00
105 ALA CA	-0.83	47.87	88.50	15.00
105 ALA C	0.53	48.36	88.97	15.00
105 ALA O	1.06	49.35	88.44	15.00
105 ALA CB	-0.67	46.68	87.59	15.00
106 LYS N	1.07	47.69	90.00	15.00
106 LYS CA	2.39	48.03	90.56	15.00
106 LYS C	3.24	46.76	90.62	15.00
106 LYS O	2.73	45.65	90.44	15.00
106 LYS CB	2.24	48.66	91.95	15.00
106 LYS CG	1.78	50.12	91.94	15.00
106 LYS CD	1.32	50.56	93.31	15.00
106 LYS CE	2.44	50.52	94.34	15.00
106 LYS NZ	3.48	51.56	94.06	15.00
107 CYS N	4.54	46.92	90.90	15.00
107 CYS CA	5.42	45.76	90.90	15.00
107 CYS C	6.51	45.83	91.97	15.00
107 CYS O	7.16	46.86	92.14	15.00
107 CYS CB	6.07	45.65	89.52	15.00
107 CYS SG	6.62	44.03	89.03	15.00
108 ARG N	6.70	44.73	92.69	15.00
108 ARG CA	7.71	44.62	93.74	15.00
108 ARG C	8.93	43.86	93.19	15.00
108 ARG O	9.61	43.14	93.93	15.00
108 ARG CB	7.16	43.87	94.96	15.00
108 ARG CG	6.08	44.58	95.79	15.00
108 ARG CD	5.41	43.58	96.74	15.00
108 ARG NE	6.38	42.60	97.25	15.00
108 ARG CZ	6.16	41.29	97.39	15.00
108 ARG NH1	4.99	40.74	97.08	15.00
108 ARG NH2	7.16	40.52	97.80	15.00
109 GLY N	9.21	44.02	91.90	15.00
109 GLY CA	10.34	43.34	91.30	15.00
109 GLY C	9.92	42.13	90.50	15.00
109 GLY O	8.77	42.01	90.10	15.00
110 TYR N	10.86	41.22	90.29	15.00
110 TYR CA	10.59	39.99	89.54	15.00
110 TYR C	11.44	38.82	90.02	15.00
110 TYR O	12.41	38.99	90.75	15.00
110 TYR CB	10.85	40.21	88.05	15.00
110 TYR CG	12.30	40.42	87.70	15.00
110 TYR CD1	13.13	39.33	87.46	15.00
110 TYR CD2	12.82	41.70	87.58	15.00
110 TYR CE1	14.46	39.52	87.10	15.00

TABLE I

110 TYR CE2	14.14	41.89	87.22	15.00
110 TYR CZ	14.95	40.80	86.98	15.00
110 TYR OH	16.25	40.99	86.61	15.00
111 ARG N	11.13	37.63	89.52	15.00
111 ARG CA	11.87	36.45	89.91	15.00
111 ARG C	11.88	35.46	88.75	15.00
111 ARG O	10.90	35.34	88.03	15.00
111 ARG CB	11.23	35.85	91.16	15.00
111 ARG CG	12.14	34.90	91.88	15.00
111 ARG CD	11.70	34.66	93.31	15.00
111 ARG NE	12.85	34.20	94.09	15.00
111 ARG CZ	13.87	34.98	94.44	15.00
111 ARG NH1	13.87	36.28	94.12	15.00
111 ARG NH2	14.89	34.48	95.13	15.00
112 GLU N	13.00	34.76	88.58	15.00
112 GLU CA	13.15	33.79	87.50	15.00
112 GLU C	13.25	32.35	87.94	15.00
112 GLU O	13.55	32.06	89.11	15.00
112 GLU CB	14.38	34.11	86.66	15.00
112 GLU CG	14.35	35.49	86.11	15.00
112 GLU CD	15.46	35.72	85.14	15.00
112 GLU OE1	15.30	35.30	83.97	15.00
112 GLU OE2	16.49	36.31	85.56	15.00
113 ILE N	12.98	31.46	86.99	15.00
113 ILE CA	13.02	30.03	87.20	15.00
113 ILE C	14.46	29.65	86.91	15.00
113 ILE O	15.13	30.34	86.15	15.00
113 ILE CB	12.04	29.30	86.23	15.00
113 ILE CG1	10.60	29.50	86.70	15.00
113 ILE CG2	12.36	27.81	86.13	15.00
113 ILE CD1	10.10	30.93	86.65	15.00
114 PRO N	15.01	28.64	87.60	15.00
114 PRO CA	16.40	28.30	87.29	15.00
114 PRO C	16.50	27.74	85.87	15.00
114 PRO O	15.74	26.85	85.48	15.00
114 PRO CB	16.77	27.29	88.39	15.00
114 PRO CG	15.46	26.66	88.76	15.00
114 PRO CD	14.52	27.85	88.75	15.00
115 GLU N	17.41	28.32	85.09	15.00
115 GLU CA	17.61	27.97	83.68	15.00
115 GLU C	17.55	26.49	83.35	15.00
115 GLU O	18.36	25.70	83.84	15.00
115 GLU CB	18.93	28.56	83.15	15.00
115 GLU CG	18.92	30.09	82.86	15.00

TABLE I

115	GLU	CD	20.11	30.56	81.97	15.00
115	GLU	OE1	20.75	29.70	81.31	15.00
115	GLU	OE2	20.39	31.79	81.92	15.00
116	GLY	N	16.55	26.11	82.56	15.00
116	GLY	CA	16.41	24.74	82.12	15.00
116	GLY	C	15.76	23.78	83.08	15.00
116	GLY	O	15.81	22.56	82.88	15.00
117	ASN	N	15.13	24.31	84.11	15.00
117	ASN	CA	14.47	23.47	85.10	15.00
117	ASN	C	12.97	23.47	84.87	15.00
117	ASN	O	12.28	24.43	85.22	15.00
117	ASN	CB	14.77	23.97	86.51	15.00
117	ASN	CG	14.21	23.05	87.58	15.00
117	ASN	OD1	13.32	22.23	87.32	15.00
117	ASN	ND2	14.72	23.19	88.80	15.00
118	GLU	N	12.47	22.38	84.29	15.00
118	GLU	CA	11.05	22.27	84.03	15.00
118	GLU	C	10.22	22.01	85.27	15.00
118	GLU	O	9.16	22.60	85.42	15.00
118	GLU	CB	10.75	21.20	82.99	15.00
118	GLU	CG	10.96	21.66	81.56	15.00
118	GLU	CD	10.34	20.72	80.56	15.00
118	GLU	OE1	9.11	20.82	80.33	15.00
118	GLU	OE2	11.08	19.88	80.01	15.00
119	LYS	N	10.73	21.18	86.18	15.00
119	LYS	CA	10.00	20.87	87.41	15.00
119	LYS	C	9.79	22.11	88.28	15.00
119	LYS	O	8.78	22.21	88.98	15.00
119	LYS	CB	10.68	19.76	88.21	15.00
119	LYS	CG	9.94	18.40	88.14	15.00
119	LYS	CD	10.13	17.64	86.81	15.00
119	LYS	CE	9.28	16.35	86.76	15.00
119	LYS	NZ	9.62	15.29	87.79	15.00
120	ALA	N	10.73	23.04	88.21	15.00
120	ALA	CA	10.61	24.30	88.94	15.00
120	ALA	C	9.57	25.15	88.23	15.00
120	ALA	O	8.72	25.75	88.88	15.00
120	ALA	CB	11.93	25.04	88.99	15.00
121	LEU	N	9.62	25.19	86.89	15.00
121	LEU	CA	8.66	25.96	86.09	15.00
121	LEU	C	7.23	25.51	86.39	15.00
121	LEU	O	6.34	26.34	86.52	15.00
121	LEU	CB	8.94	25.82	84.58	15.00
121	LEU	CG	7.91	26.43	83.60	15.00

TABLE I

121 LEU CD1	8.09	27.93	83.52	15.00
121 LEU CD2	8.08	25.84	82.22	15.00
122 LYS N	7.02	24.21	86.51	15.00
122 LYS CA	5.69	23.70	86.81	15.00
122 LYS C	5.24	24.18	88.19	15.00
122 LYS O	4.07	24.52	88.38	15.00
122 LYS CB	5.66	22.17	86.76	15.00
122 LYS CG	4.31	21.58	87.17	15.00
122 LYS CD	4.36	20.07	87.30	15.00
122 LYS CE	5.50	19.63	88.22	15.00
122 LYS NZ	5.63	18.14	88.27	15.00
123 ARG N	6.16	24.19	89.15	15.00
123 ARG CA	5.84	24.63	90.51	15.00
123 ARG C	5.51	26.11	90.47	15.00
123 ARG O	4.53	26.54	91.07	15.00
123 ARG CB	6.99	24.36	91.49	15.00
123 ARG CG	7.32	22.88	91.65	15.00
123 ARG CD	8.14	22.58	92.89	15.00
123 ARG NE	9.59	22.54	92.68	15.00
123 ARG CZ	10.40	23.60	92.76	15.00
123 ARG NH1	9.92	24.80	93.04	15.00
123 ARG NH2	11.71	23.43	92.63	15.00
124 ALA N	6.30	26.87	89.73	15.00
124 ALA CA	6.09	28.30	89.58	15.00
124 ALA C	4.72	28.57	88.98	15.00
124 ALA O	3.98	29.41	89.47	15.00
124 ALA CB	7.19	28.91	88.71	15.00
125 VAL N	4.37	27.84	87.92	15.00
125 VAL CA	3.07	28.02	87.28	15.00
125 VAL C	1.95	27.63	88.24	15.00
125 VAL O	0.88	28.23	88.22	15.00
125 VAL CB	2.96	27.17	85.98	15.00
125 VAL CG1	1.52	27.07	85.51	15.00
125 VAL CG2	3.78	27.79	84.88	15.00
126 ALA N	2.21	26.64	89.08	15.00
126 ALA CA	1.22	26.16	90.04	15.00
126 ALA C	1.10	26.92	91.36	15.00
126 ALA O	0.03	26.95	91.97	15.00
126 ALA CB	1.43	24.68	90.31	15.00
127 ARG N	2.20	27.51	91.82	15.00
127 ARG CA	2.21	28.25	93.07	15.00
127 ARG C	1.97	29.74	92.86	15.00
127 ARG O	1.45	30.43	93.75	15.00
127 ARG CB	3.55	28.07	93.81	15.00

TABLE I

127 ARG CG	3.44	27.25	95.07	15.00
127 ARG CD	3.83	25.82	94.84	15.00
127 ARG NE	5.24	25.57	95.18	15.00
127 ARG CZ	5.76	24.37	95.39	15.00
127 ARG NH1	5.03	23.27	95.29	15.00
127 ARG NH2	7.04	24.27	95.69	15.00
128 VAL N	2.38	30.23	91.69	15.00
128 VAL CA	2.22	31.64	91.36	15.00
128 VAL C	1.08	31.86	90.37	15.00
128 VAL O	0.06	32.47	90.67	15.00
128 VAL CB	3.53	32.20	90.78	15.00
128 VAL CG1	3.48	33.72	90.75	15.00
128 VAL CG2	4.72	31.71	91.58	15.00
129 GLY N	1.27	31.35	89.16	15.00
129 GLY CA	0.26	31.49	88.14	15.00
129 GLY C	0.98	31.73	86.84	15.00
129 GLY O	2.11	31.28	86.67	15.00
130 PRO N	0.36	32.47	85.91	15.00
130 PRO CA	0.96	32.76	84.62	15.00
130 PRO C	2.37	33.32	84.72	15.00
130 PRO O	2.60	34.37	85.32	15.00
130 PRO CB	-0.03	33.76	84.02	15.00
130 PRO CG	-1.33	33.27	84.53	15.00
130 PRO CD	-1.00	33.01	85.99	15.00
131 VAL N	3.32	32.57	84.15	15.00
131 VAL CA	4.72	32.96	84.13	15.00
131 VAL C	5.09	33.29	82.67	15.00
131 VAL O	4.48	32.77	81.73	15.00
131 VAL CB	5.63	31.83	84.73	15.00
131 VAL CG1	5.57	30.58	83.89	15.00
131 VAL CG2	7.07	32.28	84.86	15.00
132 SER N	6.03	34.23	82.49	15.00
132 SER CA	6.49	34.64	81.17	15.00
132 SER C	7.58	33.70	80.71	15.00
132 SER O	8.60	33.56	81.40	15.00
132 SER CB	7.08	36.05	81.25	15.00
132 SER OG	6.16	36.98	81.80	15.00
133 VAL N	7.39	33.03	79.58	15.00
133 VAL CA	8.39	32.10	79.03	15.00
133 VAL C	8.84	32.58	77.67	15.00
133 VAL O	8.20	33.43	77.06	15.00
133 VAL CB	7.86	30.66	78.87	15.00
133 VAL CG1	8.20	29.83	80.07	15.00
133 VAL CG2	6.37	30.65	78.66	15.00

TABLE I

134 ALA N	9.98	32.08	77.21	15.00
134 ALA CA	10.51	32.42	75.89	15.00
134 ALA C	10.71	31.08	75.20	15.00
134 ALA O	10.94	30.09	75.89	15.00
134 ALA CB	11.81	33.16	76.01	15.00
135 ILE N	10.58	31.02	73.88	15.00
135 ILE CA	10.74	29.75	73.17	15.00
135 ILE C	11.25	29.93	71.74	15.00
135 ILE O	11.54	31.04	71.29	15.00
135 ILE CB	9.39	29.00	73.05	15.00
135 ILE CG1	8.32	29.93	72.47	15.00
135 ILE CG2	8.98	28.39	74.37	15.00
135 ILE CD1	7.01	29.26	72.13	15.00
136 ASP N	11.37	28.80	71.04	15.00
136 ASP CA	11.80	28.77	69.65	15.00
136 ASP C	10.54	28.58	68.80	15.00
136 ASP O	10.02	27.47	68.67	15.00
136 ASP CB	12.79	27.62	69.36	15.00
136 ASP CG	13.23	27.57	67.89	15.00
136 ASP OD1	13.18	28.61	67.20	15.00
136 ASP OD2	13.64	26.49	67.41	15.00
137 ALA N	10.05	29.68	68.24	15.00
137 ALA CA	8.87	29.65	67.41	15.00
137 ALA C	9.23	29.70	65.91	15.00
137 ALA O	8.38	30.00	65.07	15.00
137 ALA CB	7.97	30.81	67.79	15.00
138 SER N	10.47	29.35	65.57	15.00
138 SER CA	10.91	29.38	64.18	15.00
138 SER C	10.40	28.27	63.28	15.00
138 SER O	10.47	28.39	62.06	15.00
138 SER CB	12.43	29.40	64.10	15.00
138 SER OG	12.93	30.59	64.68	15.00
139 LEU N	9.85	27.22	63.87	15.00
139 LEU CA	9.36	26.07	63.12	15.00
139 LEU C	8.06	26.32	62.36	15.00
139 LEU O	7.07	26.74	62.94	15.00
139 LEU CB	9.17	24.86	64.04	15.00
139 LEU CG	10.27	24.49	65.02	15.00
139 LEU CD1	11.61	24.35	64.30	15.00
139 LEU CD2	10.33	25.54	66.14	15.00
140 THR N	8.06	26.00	61.06	15.00
140 THR CA	6.87	26.19	60.24	15.00
140 THR C	5.73	25.38	60.86	15.00
140 THR O	4.56	25.75	60.77	15.00

TABLE I

140	THR	CB	7.09	25.72	58.78	15.00
140	THR	OG1	8.35	26.21	58.30	15.00
140	THR	CG2	6.00	26.29	57.88	15.00
141	SER	N	6.11	24.29	61.54	15.00
141	SER	CA	5.14	23.42	62.20	15.00
141	SER	C	4.49	24.13	63.38	15.00
141	SER	O	3.32	23.91	63.69	15.00
141	SER	CB	5.83	22.12	62.64	15.00
141	SER	OG	7.14	22.36	63.15	15.00
142	PHE	N	5.25	25.01	64.02	15.00
142	PHE	CA	4.74	25.76	65.15	15.00
142	PHE	C	3.80	26.83	64.66	15.00
142	PHE	O	2.78	27.12	65.30	15.00
142	PHE	CB	5.88	26.41	65.94	15.00
142	PHE	CG	5.41	27.24	67.09	15.00
142	PHE	CD1	5.07	28.58	66.91	15.00
142	PHE	CD2	5.31	26.70	68.37	15.00
142	PHE	CE1	4.64	29.36	67.97	15.00
142	PHE	CE2	4.89	27.47	69.44	15.00
142	PHE	CZ	4.55	28.81	69.24	15.00
143	GLN	N	4.13	27.43	63.52	15.00
143	GLN	CA	3.31	28.49	62.99	15.00
143	GLN	C	1.93	28.03	62.57	15.00
143	GLN	O	0.95	28.72	62.84	15.00
143	GLN	CB	4.05	29.25	61.89	15.00
143	GLN	CG	5.12	30.14	62.48	15.00
143	GLN	CD	6.22	30.52	61.51	15.00
143	GLN	OE1	5.97	31.14	60.47	15.00
143	GLN	NE2	7.45	30.19	61.86	15.00
144	PHE	N	1.84	26.82	62.00	15.00
144	PHE	CA	0.54	26.30	61.57	15.00
144	PHE	C	-0.14	25.30	62.52	15.00
144	PHE	O	-1.02	24.53	62.12	15.00
144	PHE	CB	0.56	25.79	60.11	15.00
144	PHE	CG	1.57	24.68	59.84	15.00
144	PHE	CD1	1.63	23.54	60.63	15.00
144	PHE	CD2	2.40	24.75	58.73	15.00
144	PHE	CE1	2.50	22.49	60.32	15.00
144	PHE	CE2	3.27	23.71	58.42	15.00
144	PHE	CZ	3.32	22.58	59.22	15.00
145	TYR	N	0.27	25.33	63.79	15.00
145	TYR	CA	-0.30	24.45	64.81	15.00
145	TYR	C	-1.80	24.73	64.93	15.00
145	TYR	O	-2.22	25.89	64.92	15.00

TABLE I

145 TYR CB	0.36	24.72	66.17	15.00
145 TYR CG	-0.43	24.13	67.33	15.00
145 TYR CD1	-0.28	22.79	67.70	15.00
145 TYR CD2	-1.38	24.90	68.01	15.00
145 TYR CE1	-1.05	22.23	68.70	15.00
145 TYR CE2	-2.15	24.35	69.01	15.00
145 TYR CZ	-1.99	23.01	69.35	15.00
145 TYR OH	-2.76	22.46	70.34	15.00
146 SER N	-2.60	23.68	65.08	15.00
146 SER CA	-4.04	23.84	65.20	15.00
146 SER C	-4.65	22.98	66.30	15.00
146 SER O	-5.72	23.29	66.81	15.00
146 SER CB	-4.74	23.59	63.84	15.00
146 SER OG	-4.46	22.30	63.31	15.00
147 LYS N	-3.96	21.91	66.67	15.00
147 LYS CA	-4.48	21.04	67.73	15.00
147 LYS C	-3.46	20.00	68.23	15.00
147 LYS O	-2.52	19.67	67.51	15.00
147 LYS CB	-5.79	20.37	67.27	15.00
147 LYS CG	-5.76	19.70	65.88	15.00
147 LYS CD	-7.11	19.05	65.50	15.00
147 LYS CE	-7.19	18.65	64.01	15.00
147 LYS NZ	-7.28	19.82	63.07	15.00
148 GLY N	-3.63	19.55	69.48	15.00
148 GLY CA	-2.75	18.55	70.07	15.00
148 GLY C	-1.56	19.09	70.85	15.00
148 GLY O	-1.43	20.29	71.06	15.00
149 VAL N	-0.71	18.18	71.31	15.00
149 VAL CA	0.50	18.54	72.07	15.00
149 VAL C	1.66	18.70	71.06	15.00
149 VAL O	2.06	17.74	70.39	15.00
149 VAL CB	0.83	17.46	73.14	15.00
149 VAL CG1	2.06	17.86	73.93	15.00
149 VAL CG2	-0.34	17.26	74.08	15.00
150 TYR N	2.21	19.90	70.99	15.00
150 TYR CA	3.25	20.21	70.03	15.00
150 TYR C	4.60	19.64	70.34	15.00
150 TYR O	5.26	20.08	71.28	15.00
150 TYR CB	3.39	21.72	69.86	15.00
150 TYR CG	4.42	22.11	68.81	15.00
150 TYR CD1	4.39	21.53	67.54	15.00
150 TYR CD2	5.44	23.02	69.11	15.00
150 TYR CE1	5.36	21.85	66.58	15.00
150 TYR CE2	6.41	23.33	68.15	15.00

TABLE I

150	TYR	CZ	6.37	22.74	66.90	15.00
150	TYR	OH	7.34	23.02	65.97	15.00
151	TYR	N	5.03	18.69	69.53	15.00
151	TYR	CA	6.35	18.11	69.70	15.00
151	TYR	C	7.09	18.15	68.37	15.00
151	TYR	O	6.65	17.56	67.39	15.00
151	TYR	CB	6.30	16.68	70.20	15.00
151	TYR	CG	7.67	16.22	70.63	15.00
151	TYR	CD1	8.45	17.02	71.46	15.00
151	TYR	CD2	8.20	15.02	70.17	15.00
151	TYR	CE1	9.74	16.65	71.82	15.00
151	TYR	CE2	9.50	14.63	70.52	15.00
151	TYR	CZ	10.26	15.45	71.35	15.00
151	TYR	OH	11.55	15.08	71.70	15.00
152	ASP	N	8.21	18.85	68.35	15.00
152	ASP	CA	8.98	18.96	67.12	15.00
152	ASP	C	10.47	18.82	67.44	15.00
152	ASP	O	11.08	19.72	68.03	15.00
152	ASP	CB	8.70	20.31	66.45	15.00
152	ASP	CG	9.22	20.37	65.03	15.00
152	ASP	OD1	8.48	19.96	64.12	15.00
152	ASP	OD2	10.37	20.82	64.82	15.00
153	GLU	N	11.03	17.68	67.05	15.00
153	GLU	CA	12.44	17.38	67.31	15.00
153	GLU	C	13.40	18.37	66.69	15.00
153	GLU	O	14.59	18.34	66.98	15.00
153	GLU	CB	12.76	15.94	66.86	15.00
153	GLU	CG	12.29	15.56	65.44	15.00
153	GLU	CD	13.28	15.95	64.33	15.00
153	GLU	OE1	14.38	15.36	64.28	15.00
153	GLU	OE2	12.95	16.84	63.50	15.00
154	SER	N	12.89	19.26	65.85	15.00
154	SER	CA	13.75	20.24	65.20	15.00
154	SER	C	13.86	21.54	66.01	15.00
154	SER	O	14.71	22.38	65.71	15.00
154	SER	CB	13.20	20.54	63.80	15.00
154	SER	OG	14.08	21.32	63.02	15.00
155	CYS	N	13.02	21.69	67.03	15.00
155	CYS	CA	13.01	22.90	67.86	15.00
155	CYS	C	14.34	23.17	68.55	15.00
155	CYS	O	14.74	22.42	69.45	15.00
155	CYS	CB	11.86	22.85	68.87	15.00
155	CYS	SG	11.05	24.47	69.10	15.00
156	ASN	N	15.02	24.23	68.14	15.00

TABLE I

156 ASN CA	16.33	24.57	68.70	15.00
156 ASN C	16.29	25.23	70.07	15.00
156 ASN O	16.21	26.46	70.19	15.00
156 ASN CB	17.16	25.40	67.73	15.00
156 ASN CG	18.54	25.71	68.28	15.00
156 ASN OD1	18.89	26.86	68.48	15.00
156 ASN ND2	19.32	24.66	68.57	15.00
157 SER N	16.46	24.39	71.09	15.00
157 SER CA	16.46	24.79	72.50	15.00
157 SER C	17.39	25.95	72.87	15.00
157 SER O	17.24	26.54	73.94	15.00
157 SER CB	16.79	23.56	73.34	15.00
157 SER OG	16.11	22.42	72.84	15.00
158 ASP N	18.34	26.27	71.99	15.00
158 ASP CA	19.29	27.35	72.24	15.00
158 ASP C	18.88	28.70	71.64	15.00
158 ASP O	19.31	29.76	72.09	15.00
158 ASP CB	20.69	26.96	71.75	15.00
158 ASP CG	21.57	26.39	72.87	15.00
158 ASP OD1	21.02	25.82	73.85	15.00
158 ASP OD2	22.82	26.53	72.78	15.00
159 ASN N	18.07	28.66	70.59	15.00
159 ASN CA	17.63	29.89	69.97	15.00
159 ASN C	16.22	30.22	70.46	15.00
159 ASN O	15.25	29.58	70.04	15.00
159 ASN CB	17.69	29.76	68.45	15.00
159 ASN CG	16.80	30.75	67.73	15.00
159 ASN OD1	16.93	31.98	67.88	15.00
159 ASN ND2	15.86	30.22	66.96	15.00
160 LEU N	16.13	31.16	71.39	15.00
160 LEU CA	14.83	31.58	71.93	15.00
160 LEU C	14.48	32.83	71.16	15.00
160 LEU O	15.25	33.79	71.14	15.00
160 LEU CB	14.90	31.88	73.44	15.00
160 LEU CG	15.29	30.75	74.43	15.00
160 LEU CD1	15.63	31.34	75.78	15.00
160 LEU CD2	14.20	29.70	74.54	15.00
161 ASN N	13.32	32.82	70.51	15.00
161 ASN CA	12.91	33.94	69.69	15.00
161 ASN C	11.44	34.33	69.76	15.00
161 ASN O	10.94	34.97	68.85	15.00
161 ASN CB	13.25	33.62	68.24	15.00
161 ASN CG	12.59	32.35	67.78	15.00
161 ASN OD1	11.36	32.28	67.67	15.00

TABLE I

161 ASN ND2	13.38	31.31	67.58	15.00
162 HIS N	10.72	33.90	70.78	15.00
162 HIS CA	9.33	34.31	70.87	15.00
162 HIS C	8.84	34.19	72.29	15.00
162 HIS O	8.74	33.09	72.84	15.00
162 HIS CB	8.45	33.51	69.91	15.00
162 HIS CG	7.10	34.12	69.68	15.00
162 HIS ND1	6.93	35.47	69.42	15.00
162 HIS CD2	5.86	33.58	69.66	15.00
162 HIS CE1	5.64	35.72	69.24	15.00
162 HIS NE2	4.97	34.59	69.38	15.00
163 ALA N	8.58	35.35	72.90	15.00
163 ALA CA	8.09	35.40	74.26	15.00
163 ALA C	6.63	34.98	74.30	15.00
163 ALA O	5.78	35.55	73.61	15.00
163 ALA CB	8.27	36.79	74.81	15.00
164 VAL N	6.36	33.96	75.09	15.00
164 VAL CA	5.02	33.43	75.28	15.00
164 VAL C	4.69	33.44	76.78	15.00
164 VAL O	5.54	33.79	77.60	15.00
164 VAL CB	4.95	32.00	74.70	15.00
164 VAL CG1	5.97	31.10	75.37	15.00
164 VAL CG2	3.57	31.44	74.89	15.00
165 LEU N	3.45	33.09	77.15	15.00
165 LEU CA	3.04	33.03	78.55	15.00
165 LEU C	2.46	31.67	78.88	15.00
165 LEU O	1.65	31.15	78.12	15.00
165 LEU CB	1.96	34.09	78.85	15.00
165 LEU CG	1.43	34.18	80.29	15.00
165 LEU CD1	2.39	34.99	81.12	15.00
165 LEU CD2	0.06	34.82	80.33	15.00
166 ALA N	2.87	31.11	80.01	15.00
166 ALA CA	2.35	29.81	80.46	15.00
166 ALA C	1.08	30.09	81.24	15.00
166 ALA O	1.06	30.96	82.11	15.00
166 ALA CB	3.36	29.12	81.34	15.00
167 VAL N	0.02	29.38	80.89	15.00
167 VAL CA	-1.29	29.54	81.52	15.00
167 VAL C	-1.67	28.28	82.34	15.00
167 VAL O	-2.71	28.21	83.00	15.00
167 VAL CB	-2.32	29.91	80.40	15.00
167 VAL CG1	-3.67	29.28	80.59	15.00
167 VAL CG2	-2.45	31.41	80.33	15.00
168 GLY N	-0.76	27.32	82.38	15.00

TABLE I

168 GLY CA	-0.99	26.12	83.13	15.00
168 GLY C	-0.16	24.99	82.57	15.00
168 GLY O	0.86	25.22	81.93	15.00
169 TYR N	-0.61	23.78	82.81	15.00
169 TYR CA	0.05	22.58	82.33	15.00
169 TYR C	-1.02	21.51	82.42	15.00
169 TYR O	-2.11	21.76	82.93	15.00
169 TYR CB	1.27	22.22	83.20	15.00
169 TYR CG	1.02	22.11	84.70	15.00
169 TYR CD1	0.52	20.94	85.28	15.00
169 TYR CD2	1.32	23.18	85.56	15.00
169 TYR CE1	0.32	20.84	86.66	15.00
169 TYR CE2	1.12	23.08	86.94	15.00
169 TYR CZ	0.62	21.91	87.48	15.00
169 TYR OH	0.44	21.83	88.85	15.00
170 GLY N	-0.71	20.33	81.90	15.00
170 GLY CA	-1.65	19.23	81.94	15.00
170 GLY C	-1.16	18.11	81.05	15.00
170 GLY O	-0.03	18.14	80.54	15.00
171 ILE N	-2.04	17.15	80.81	15.00
171 ILE CA	-1.78	15.98	79.97	15.00
171 ILE C	-2.96	15.87	79.00	15.00
171 ILE O	-3.95	16.60	79.14	15.00
171 ILE CB	-1.62	14.73	80.86	15.00
171 ILE CG1	-1.47	13.46	80.02	15.00
171 ILE CG2	-2.76	14.65	81.87	15.00
171 ILE CD1	-1.03	12.22	80.81	15.00
172 GLN N	-2.86	15.03	77.96	15.00
172 GLN CA	-3.97	14.90	77.01	15.00
172 GLN C	-4.16	13.50	76.45	15.00
172 GLN O	-5.04	12.76	76.88	15.00
172 GLN CB	-3.79	15.89	75.87	15.00
172 GLN CG	-4.95	15.94	74.92	15.00
172 GLN CD	-4.83	17.08	73.95	15.00
172 GLN OE1	-3.81	17.24	73.28	15.00
172 GLN NE2	-5.86	17.91	73.88	15.00
173 LYS N	-3.39	13.15	75.44	15.00
173 LYS CA	-3.51	11.81	74.89	15.00
173 LYS C	-2.36	11.09	75.55	15.00
173 LYS O	-1.55	10.43	74.90	15.00
173 LYS CB	-3.36	11.82	73.36	15.00
173 LYS CG	-4.57	12.39	72.60	15.00
173 LYS CD	-5.81	11.53	72.82	15.00
173 LYS CE	-7.06	12.17	72.19	15.00

TABLE I

173 LYS NZ	-8.35	11.45	72.50	15.00
174 GLY N	-2.29	11.24	76.87	15.00
174 GLY CA	-1.20	10.64	77.60	15.00
174 GLY C	0.03	11.49	77.36	15.00
174 GLY O	1.17	11.08	77.62	15.00
175 ASN N	-0.19	12.72	76.92	15.00
175 ASN CA	0.93	13.59	76.64	15.00
175 ASN C	1.02	14.78	77.57	15.00
175 ASN O	0.07	15.56	77.70	15.00
175 ASN CB	0.88	14.04	75.18	15.00
175 ASN CG	0.72	12.87	74.20	15.00
175 ASN OD1	-0.28	12.77	73.49	15.00
175 ASN ND2	1.71	11.97	74.19	15.00
176 LYS N	2.15	14.88	78.27	15.00
176 LYS CA	2.42	15.97	79.20	15.00
176 LYS C	2.40	17.22	78.34	15.00
176 LYS O	2.76	17.17	77.16	15.00
176 LYS CB	3.83	15.84	79.78	15.00
176 LYS CG	4.38	14.45	79.93	15.00
176 LYS CD	4.27	13.97	81.36	15.00
176 LYS CE	4.98	12.63	81.55	15.00
176 LYS NZ	4.97	12.14	82.96	15.00
177 HIS N	2.01	18.36	78.91	15.00
177 HIS CA	1.99	19.58	78.13	15.00
177 HIS C	1.88	20.86	78.95	15.00
177 HIS O	1.47	20.84	80.12	15.00
177 HIS CB	0.88	19.53	77.06	15.00
177 HIS CG	-0.52	19.66	77.59	15.00
177 HIS ND1	-1.43	18.63	77.56	15.00
177 HIS CD2	-1.16	20.71	78.16	15.00
177 HIS CE1	-2.57	19.03	78.08	15.00
177 HIS NE2	-2.44	20.29	78.45	15.00
178 TRP N	2.25	21.96	78.31	15.00
178 TRP CA	2.17	23.29	78.89	15.00
178 TRP C	1.16	24.04	78.03	15.00
178 TRP O	1.20	23.95	76.79	15.00
178 TRP CB	3.52	23.99	78.78	15.00
178 TRP CG	4.66	23.32	79.46	15.00
178 TRP CD1	5.71	22.70	78.87	15.00
178 TRP CD2	4.94	23.34	80.86	15.00
178 TRP NE1	6.65	22.35	79.80	15.00
178 TRP CE2	6.21	22.73	81.03	15.00
178 TRP CE3	4.26	23.83	81.99	15.00
178 TRP CZ2	6.80	22.60	82.29	15.00

TABLE I

178 TRP CZ3	4.85	23.70	83.23	15.00
178 TRP CH2	6.12	23.09	83.38	15.00
179 ILE N	0.22	24.75	78.66	15.00
179 ILE CA	-0.79	25.51	77.92	15.00
179 ILE C	-0.20	26.89	77.64	15.00
179 ILE O	-0.07	27.71	78.54	15.00
179 ILE CB	-2.08	25.66	78.74	15.00
179 ILE CG1	-2.67	24.27	79.03	15.00
179 ILE CG2	-3.07	26.56	78.02	15.00
179 ILE CD1	-3.80	24.25	80.04	15.00
180 ILE N	0.21	27.09	76.39	15.00
180 ILE CA	0.83	28.33	75.96	15.00
180 ILE C	-0.17	29.28	75.34	15.00
180 ILE O	-1.09	28.85	74.65	15.00
180 ILE CB	1.99	28.05	74.99	15.00
180 ILE CG1	3.32	28.14	75.72	15.00
180 ILE CG2	1.97	28.97	73.83	15.00
180 ILE CD1	3.53	27.06	76.73	15.00
181 LYS N	0.00	30.57	75.64	15.00
181 LYS CA	-0.85	31.66	75.14	15.00
181 LYS C	-0.01	32.55	74.22	15.00
181 LYS O	0.91	33.23	74.68	15.00
181 LYS CB	-1.38	32.51	76.30	15.00
181 LYS CG	-2.27	33.66	75.84	15.00
181 LYS CD	-2.51	34.72	76.91	15.00
181 LYS CE	-3.38	35.84	76.37	15.00
181 LYS NZ	-3.58	36.94	77.35	15.00
182 ASN N	-0.32	32.56	72.93	15.00
182 ASN CA	0.44	33.36	71.97	15.00
182 ASN C	-0.18	34.74	71.73	15.00
182 ASN O	-1.29	35.00	72.17	15.00
182 ASN CB	0.55	32.59	70.66	15.00
182 ASN CG	1.83	32.87	69.93	15.00
182 ASN OD1	2.41	33.95	70.05	15.00
182 ASN ND2	2.31	31.89	69.17	15.00
183 SER N	0.55	35.64	71.08	15.00
183 SER CA	0.03	36.98	70.82	15.00
183 SER C	-0.32	37.19	69.34	15.00
183 SER O	-0.25	38.31	68.82	15.00
183 SER CB	1.03	38.04	71.25	15.00
183 SER OG	2.31	37.80	70.69	15.00
184 TRP N	-0.74	36.12	68.68	15.00
184 TRP CA	-1.05	36.18	67.26	15.00
184 TRP C	-2.53	36.23	66.88	15.00

TABLE I

184	TRP	O	-2.87	36.09	65.71	15.00
184	TRP	CB	-0.36	35.01	66.55	15.00
184	TRP	CG	1.12	35.12	66.54	15.00
184	TRP	CD1	1.85	36.23	66.82	15.00
184	TRP	CD2	2.05	34.09	66.23	15.00
184	TRP	NE1	3.18	35.97	66.69	15.00
184	TRP	CE2	3.34	34.66	66.33	15.00
184	TRP	CE3	1.94	32.75	65.87	15.00
184	TRP	CZ2	4.51	33.92	66.09	15.00
184	TRP	CZ3	3.10	32.01	65.63	15.00
184	TRP	CH2	4.37	32.60	65.74	15.00
185	GLY	N	-3.40	36.48	67.85	15.00
185	GLY	CA	-4.82	36.54	67.56	15.00
185	GLY	C	-5.46	35.18	67.75	15.00
185	GLY	O	-4.75	34.16	67.80	15.00
186	GLU	N	-6.78	35.15	67.86	15.00
186	GLU	CA	-7.54	33.91	68.07	15.00
186	GLU	C	-7.53	32.99	66.85	15.00
186	GLU	O	-7.65	31.78	67.00	15.00
186	GLU	CB	-8.98	34.24	68.44	15.00
186	GLU	CG	-9.10	35.32	69.49	15.00
186	GLU	CD	-10.45	36.03	69.45	15.00
186	GLU	OE1	-10.66	36.84	68.51	15.00
186	GLU	OE2	-11.29	35.77	70.34	15.00
187	ASN	N	-7.43	33.58	65.66	15.00
187	ASN	CA	-7.43	32.78	64.42	15.00
187	ASN	C	-6.14	31.97	64.30	15.00
187	ASN	O	-6.07	31.05	63.49	15.00
187	ASN	CB	-7.64	33.68	63.19	15.00
187	ASN	CG	-8.60	33.05	62.14	15.00
187	ASN	OD1	-8.17	32.52	61.10	15.00
187	ASN	ND2	-9.90	33.18	62.38	15.00
188	TRP	N	-5.12	32.31	65.10	15.00
188	TRP	CA	-3.87	31.57	65.07	15.00
188	TRP	C	-4.06	30.34	65.95	15.00
188	TRP	O	-4.78	30.41	66.95	15.00
188	TRP	CB	-2.71	32.38	65.64	15.00
188	TRP	CG	-1.45	31.59	65.56	15.00
188	TRP	CD1	-0.68	31.41	64.46	15.00
188	TRP	CD2	-0.89	30.74	66.58	15.00
188	TRP	NE1	0.30	30.49	64.71	15.00
188	TRP	CE2	0.20	30.06	66.00	15.00
188	TRP	CE3	-1.21	30.49	67.92	15.00
188	TRP	CZ2	0.97	29.14	66.71	15.00

TABLE I

188 TRP CZ3	-0.44	29.57	68.62	15.00
188 TRP CH2	0.64	28.92	68.02	15.00
189 GLY N	-3.38	29.25	65.60	15.00
189 GLY CA	-3.46	28.02	66.36	15.00
189 GLY C	-4.84	27.67	66.87	15.00
189 GLY O	-5.86	27.96	66.24	15.00
190 ASN N	-4.87	27.07	68.04	15.00
190 ASN CA	-6.10	26.65	68.68	15.00
190 ASN C	-6.74	27.83	69.39	15.00
190 ASN O	-6.67	27.92	70.61	15.00
190 ASN CB	-5.76	25.58	69.71	15.00
190 ASN CG	-6.97	24.84	70.19	15.00
190 ASN OD1	-8.11	25.26	69.96	15.00
190 ASN ND2	-6.73	23.72	70.87	15.00
191 LYS N	-7.33	28.75	68.61	15.00
191 LYS CA	-7.97	29.96	69.14	15.00
191 LYS C	-7.01	30.82	69.95	15.00
191 LYS O	-7.36	31.36	71.00	15.00
191 LYS CB	-9.20	29.62	69.99	15.00
191 LYS CG	-10.33	28.92	69.26	15.00
191 LYS CD	-11.50	28.66	70.20	15.00
191 LYS CE	-12.26	27.39	69.82	15.00
191 LYS NZ	-11.42	26.16	70.01	15.00
192 GLY N	-5.79	30.96	69.45	15.00
192 GLY CA	-4.80	31.75	70.13	15.00
192 GLY C	-3.88	30.93	70.99	15.00
192 GLY O	-2.79	31.39	71.32	15.00
193 TYR N	-4.28	29.72	71.35	15.00
193 TYR CA	-3.43	28.86	72.18	15.00
193 TYR C	-2.80	27.69	71.45	15.00
193 TYR O	-3.25	27.27	70.39	15.00
193 TYR CB	-4.21	28.31	73.39	15.00
193 TYR CG	-4.63	29.36	74.36	15.00
193 TYR CD1	-3.77	29.78	75.37	15.00
193 TYR CD2	-5.85	30.00	74.22	15.00
193 TYR CE1	-4.12	30.82	76.22	15.00
193 TYR CE2	-6.21	31.05	75.06	15.00
193 TYR CZ	-5.34	31.45	76.06	15.00
193 TYR OH	-5.68	32.50	76.87	15.00
194 ILE N	-1.73	27.17	72.05	15.00
194 ILE CA	-1.01	26.02	71.53	15.00
194 ILE C	-0.53	25.21	72.71	15.00
194 ILE O	0.04	25.75	73.66	15.00
194 ILE CB	0.20	26.40	70.62	15.00

TABLE I

194 ILE CG1	1.05	25.15	70.32	15.00
194 ILE CG2	1.04	27.49	71.24	15.00
194 ILE CD1	2.33	25.42	69.60	15.00
195 LEU N	-0.86	23.92	72.69	15.00
195 LEU CA	-0.45	23.00	73.73	15.00
195 LEU C	0.90	22.46	73.34	15.00
195 LEU O	0.99	21.68	72.42	15.00
195 LEU CB	-1.43	21.83	73.83	15.00
195 LEU CG	-2.45	21.90	74.96	15.00
195 LEU CD1	-3.38	23.07	74.76	15.00
195 LEU CD2	-3.23	20.60	74.98	15.00
196 MET N	1.95	22.94	74.01	15.00
196 MET CA	3.31	22.50	73.75	15.00
196 MET C	3.70	21.30	74.64	15.00
196 MET O	2.97	20.96	75.57	15.00
196 MET CB	4.27	23.66	73.96	15.00
196 MET CG	4.16	24.69	72.88	15.00
196 MET SD	5.11	26.17	73.23	15.00
196 MET CE	6.79	25.64	72.90	15.00
197 ALA N	4.85	20.69	74.38	15.00
197 ALA CA	5.27	19.52	75.15	15.00
197 ALA C	5.99	19.75	76.49	15.00
197 ALA O	7.03	20.42	76.57	15.00
197 ALA CB	6.07	18.58	74.28	15.00
198 ARG N	5.43	19.14	77.54	15.00
198 ARG CA	5.99	19.22	78.88	15.00
198 ARG C	6.80	17.96	79.20	15.00
198 ARG O	6.41	16.84	78.86	15.00
198 ARG CB	4.89	19.44	79.92	15.00
198 ARG CG	5.35	19.32	81.39	15.00
198 ARG CD	4.48	20.12	82.35	15.00
198 ARG NE	3.08	19.72	82.36	15.00
198 ARG CZ	2.62	18.64	82.99	15.00
198 ARG NH1	3.46	17.86	83.66	15.00
198 ARG NH2	1.33	18.34	82.95	15.00
199 ASN N	7.96	18.18	79.83	15.00
199 ASN CA	8.87	17.11	80.24	15.00
199 ASN C	9.57	16.30	79.13	15.00
199 ASN O	10.36	15.40	79.43	15.00
199 ASN CB	8.21	16.18	81.28	15.00
199 ASN CG	8.15	16.81	82.68	15.00
199 ASN OD1	7.06	17.06	83.21	15.00
199 ASN ND2	9.31	17.07	83.27	15.00
200 LYS N	9.31	16.63	77.88	15.00

TABLE I

200 LYS CA	9.97	15.94	76.77	15.00
200 LYS C	11.29	16.67	76.54	15.00
200 LYS O	11.54	17.17	75.45	15.00
200 LYS CB	9.11	15.96	75.49	15.00
200 LYS CG	8.09	14.81	75.36	15.00
200 LYS CD	8.32	14.01	74.06	15.00
200 LYS CE	7.22	12.96	73.78	15.00
200 LYS NZ	5.87	13.49	73.41	15.00
201 ASN N	12.13	16.71	77.57	15.00
201 ASN CA	13.42	17.39	77.56	15.00
201 ASN C	13.27	18.81	77.00	15.00
201 ASN O	13.24	18.99	75.80	15.00
201 ASN CB	14.47	16.61	76.74	15.00
201 ASN CG	15.92	17.21	76.86	15.00
201 ASN OD1	16.88	16.46	77.06	15.00
201 ASN ND2	16.06	18.52	76.67	15.00
202 ASN N	13.15	19.80	77.89	15.00
202 ASN CA	13.04	21.22	77.54	15.00
202 ASN C	12.73	21.51	76.05	15.00
202 ASN O	13.56	22.10	75.34	15.00
202 ASN CB	14.35	21.92	77.95	15.00
202 ASN CG	14.13	23.30	78.56	15.00
202 ASN OD1	13.04	23.64	79.00	15.00
202 ASN ND2	15.18	24.09	78.60	15.00
203 ALA N	11.55	21.12	75.59	15.00
203 ALA H	11.67	20.72	76.05	15.00
203 ALA CA	11.15	21.27	74.19	15.00
203 ALA CB	10.97	20.66	73.61	15.00
203 ALA C	11.04	22.76	73.85	15.00
203 ALA O	10.23	23.49	74.41	15.00
204 CYS N	11.83	23.20	72.87	15.00
204 CYS CA	11.81	24.59	72.40	15.00
204 CYS C	12.38	25.57	73.42	15.00
204 CYS O	12.06	26.76	73.36	15.00
204 CYS CB	10.39	25.02	72.00	15.00
204 CYS SG	9.66	24.16	70.56	15.00
205 GLY N	13.21	25.07	74.33	15.00
205 GLY CA	13.84	25.89	75.36	15.00
205 GLY C	12.87	26.70	76.20	15.00
205 GLY O	13.17	27.80	76.64	15.00
206 ILE N	11.72	26.10	76.48	15.00
206 ILE CA	10.67	26.74	77.23	15.00
206 ILE C	11.05	27.11	78.67	15.00
206 ILE O	10.90	28.27	79.08	15.00

TABLE I

206	ILE	CB	9.41	25.86	77.17	15.00
206	ILE	CG1	8.20	26.58	77.77	15.00
206	ILE	CG2	9.69	24.53	77.81	15.00
206	ILE	CD1	6.88	25.88	77.49	15.00
207	ALA	N	11.62	26.17	79.41	15.00
207	ALA	CA	12.03	26.40	80.79	15.00
207	ALA	C	13.38	27.11	80.93	15.00
207	ALA	O	13.98	27.10	82.01	15.00
207	ALA	CB	12.05	25.09	81.54	15.00
208	ASN	N	13.84	27.74	79.86	15.00
208	ASN	CA	15.12	28.43	79.86	15.00
208	ASN	C	15.08	29.92	80.08	15.00
208	ASN	O	16.13	30.53	80.28	15.00
208	ASN	CB	15.84	28.22	78.54	15.00
208	ASN	CG	16.81	27.09	78.60	15.00
208	ASN	OD1	16.50	26.04	79.14	15.00
208	ASN	ND2	17.99	27.30	78.04	15.00
209	LEU	N	13.91	30.54	79.98	15.00
209	LEU	CA	13.84	31.98	80.18	15.00
209	LEU	C	12.65	32.45	81.02	15.00
209	LEU	O	12.23	33.63	80.94	15.00
209	LEU	CB	13.89	32.69	78.83	15.00
209	LEU	CG	14.33	34.16	78.81	15.00
209	LEU	CD1	15.60	34.32	79.63	15.00
209	LEU	CD2	14.56	34.61	77.37	15.00
210	ALA	N	12.15	31.57	81.87	15.00
210	ALA	H	12.50	30.94	81.70	15.00
210	ALA	CA	10.99	31.87	82.71	15.00
210	ALA	CB	10.41	31.04	83.16	15.00
210	ALA	C	11.33	33.00	83.69	15.00
210	ALA	O	12.46	33.21	84.13	15.00
211	SER	N	10.26	33.74	84.06	15.00
211	SER	CA	10.37	34.83	85.02	15.00
211	SER	C	8.96	35.33	85.31	15.00
211	SER	O	8.09	35.24	84.45	15.00
211	SER	CB	11.22	35.98	84.46	15.00
211	SER	OG	10.50	36.76	83.53	15.00
212	PHE	N	8.72	35.78	86.53	15.00
212	PHE	CA	7.42	36.30	86.88	15.00
212	PHE	C	7.64	37.49	87.78	15.00
212	PHE	O	8.68	37.61	88.42	15.00
212	PHE	CB	6.57	35.23	87.56	15.00
212	PHE	CG	7.23	34.60	88.75	15.00
212	PHE	CD1	7.39	35.31	89.94	15.00

TABLE I

212 PHE CD2	7.68	33.28	88.69	15.00
212 PHE CE1	7.99	34.73	91.05	15.00
212 PHE CE2	8.28	32.68	89.78	15.00
212 PHE CZ	8.44	33.41	90.97	15.00
213 PRO N	6.69	38.43	87.80	15.00
213 PRO CA	6.84	39.62	88.65	15.00
213 PRO C	6.38	39.34	90.09	15.00
213 PRO O	5.56	38.44	90.33	15.00
213 PRO CB	5.93	40.62	87.97	15.00
213 PRO CG	4.79	39.75	87.52	15.00
213 PRO CD	5.47	38.52	86.97	15.00
214 LYS N	6.96	40.05	91.04	15.00
214 LYS CA	6.57	39.89	92.42	15.00
214 LYS C	5.65	41.06	92.68	15.00
214 LYS O	6.12	42.17	92.91	15.00
214 LYS CB	7.78	39.94	93.36	15.00
214 LYS CG	8.68	38.72	93.27	15.00
214 LYS CD	9.78	38.70	94.34	15.00
214 LYS CE	10.67	39.94	94.26	15.00
214 LYS NZ	11.94	39.80	95.03	15.00
215 MET N	4.36	40.85	92.51	15.00
215 MET CA	3.39	41.91	92.77	15.00
215 MET C	2.86	41.71	94.19	15.00
215 MET CB	2.25	41.86	91.76	15.00
215 MET CG	1.06	42.74	92.12	15.00
215 MET SD	-0.32	42.54	90.98	15.00
215 MET CE	0.28	43.53	89.53	15.00

TABLE II

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for the cathepsin K complex with inhibitor 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone.

Residue Atom	X	Y	Z	B
1 ALA CB	-54.11	-32.66	67.34	15.00
1 ALA C	-54.02	-32.71	64.82	15.00
1 ALA O	-53.62	-33.85	64.58	15.00
1 ALA N	-56.02	-33.44	65.99	15.00
1 ALA CA	-54.90	-32.46	66.05	15.00
2 PRO N	-53.80	-31.67	63.99	15.00
2 PRO CD	-54.47	-30.37	64.11	15.00
2 PRO CA	-52.98	-31.72	62.76	15.00
2 PRO CB	-53.14	-30.31	62.20	15.00
2 PRO CG	-54.52	-29.90	62.67	15.00
2 PRO C	-51.51	-32.06	62.95	15.00
2 PRO O	-50.99	-32.06	64.08	15.00
3 ASP N	-50.81	-32.33	61.85	15.00
3 ASP CA	-49.39	-32.67	61.91	15.00
3 ASP CB	-49.04	-33.71	60.85	15.00
3 ASP CG	-49.27	-35.14	61.32	15.00
3 ASP OD1	-48.47	-35.61	62.17	15.00
3 ASP OD2	-50.24	-35.79	60.85	15.00
3 ASP C	-48.52	-31.44	61.73	15.00
3 ASP O	-47.93	-31.24	60.68	15.00
4 SER N	-48.41	-30.64	62.79	15.00
4 SER CA	-47.62	-29.41	62.75	15.00
4 SER CB	-48.55	-28.25	62.37	15.00
4 SER OG	-47.82	-27.08	62.01	15.00
4 SER C	-47.01	-29.13	64.12	15.00
4 SER O	-47.59	-29.49	65.15	15.00
5 VAL N	-45.83	-28.51	64.15	15.00
5 VAL CA	-45.19	-28.15	65.41	15.00
5 VAL CB	-44.36	-29.31	66.03	15.00
5 VAL CG1	-43.06	-29.53	65.29	15.00
5 VAL CG2	-44.08	-29.04	67.50	15.00
5 VAL C	-44.34	-26.88	65.24	15.00
5 VAL O	-43.64	-26.69	64.25	15.00
6 ASP N	-44.48	-25.96	66.20	15.00

TABLE II

6 ASP CA	-43.78	-24.69	66.19	15.00
6 ASP CB	-44.75	-23.59	65.74	15.00
6 ASP CG	-44.11	-22.19	65.67	15.00
6 ASP OD1	-42.99	-21.99	66.18	15.00
6 ASP OD2	-44.75	-21.27	65.13	15.00
6 ASP C	-43.37	-24.47	67.64	15.00
6 ASP O	-44.19	-24.09	68.48	15.00
7 TYR N	-42.10	-24.68	67.95	15.00
7 TYR CA	-41.65	-24.50	69.33	15.00
7 TYR CB	-40.30	-25.18	69.53	15.00
7 TYR CG	-40.41	-26.69	69.53	15.00
7 TYR CD1	-40.91	-27.37	70.64	15.00
7 TYR CE1	-41.02	-28.74	70.65	15.00
7 TYR CD2	-40.02	-27.43	68.42	15.00
7 TYR CE2	-40.13	-28.80	68.42	15.00
7 TYR CZ	-40.63	-29.45	69.53	15.00
7 TYR OH	-40.70	-30.82	69.53	15.00
7 TYR C	-41.62	-23.07	69.82	15.00
7 TYR O	-41.41	-22.81	71.00	15.00
8 ARG N	-41.83	-22.12	68.92	15.00
8 ARG CA	-41.84	-20.72	69.31	15.00
8 ARG CB	-42.00	-19.80	68.09	15.00
8 ARG CG	-40.82	-19.80	67.14	15.00
8 ARG CD	-41.13	-18.98	65.91	15.00
8 ARG NE	-42.05	-19.66	65.00	15.00
8 ARG CZ	-42.68	-19.07	64.00	15.00
8 ARG NH1	-42.49	-17.78	63.77	15.00
8 ARG NH2	-43.50	-19.77	63.22	15.00
8 ARG C	-43.00	-20.51	70.28	15.00
8 ARG O	-42.87	-19.79	71.28	15.00
9 LYS N	-44.10	-21.19	70.00	15.00
9 LYS CA	-45.30	-21.10	70.82	15.00
9 LYS CB	-46.49	-21.67	70.05	15.00
9 LYS CG	-46.76	-21.07	68.69	15.00
9 LYS CD	-48.04	-21.67	68.14	15.00
9 LYS CE	-48.28	-21.36	66.69	15.00
9 LYS NZ	-49.49	-22.07	66.19	15.00
9 LYS C	-45.20	-21.83	72.16	15.00
9 LYS O	-46.13	-21.78	72.97	15.00
10 LYS N	-44.10	-22.53	72.40	15.00
10 LYS CA	-43.92	-23.27	73.64	15.00
10 LYS CB	-43.47	-24.71	73.36	15.00
10 LYS CG	-43.75	-25.23	71.96	15.00

TABLE II

10	LYS	CD	-45.22	-25.49	71.73	15.00
10	LYS	CE	-45.52	-26.97	71.83	15.00
10	LYS	NZ	-45.21	-27.50	73.19	15.00
10	LYS	C	-42.88	-22.63	74.54	15.00
10	LYS	O	-42.67	-23.06	75.67	15.00
11	GLY	N	-42.16	-21.63	74.03	15.00
11	GLY	CA	-41.15	-20.98	74.83	15.00
11	GLY	C	-39.79	-21.63	74.68	15.00
11	GLY	O	-38.90	-21.42	75.50	15.00
12	TYR	N	-39.60	-22.38	73.60	15.00
12	TYR	CA	-38.34	-23.07	73.36	15.00
12	TYR	CB	-38.56	-24.39	72.61	15.00
12	TYR	CG	-39.12	-25.53	73.43	15.00
12	TYR	CD1	-40.27	-25.37	74.19	15.00
12	TYR	CE1	-40.82	-26.43	74.89	15.00
12	TYR	CD2	-38.53	-26.79	73.39	15.00
12	TYR	CE2	-39.08	-27.86	74.09	15.00
12	TYR	CZ	-40.23	-27.67	74.84	15.00
12	TYR	OH	-40.79	-28.71	75.55	15.00
12	TYR	C	-37.31	-22.26	72.60	15.00
12	TYR	O	-36.14	-22.61	72.57	15.00
13	VAL	N	-37.70	-21.18	71.93	15.00
13	VAL	CA	-36.72	-20.42	71.18	15.00
13	VAL	CB	-36.97	-20.48	69.67	15.00
13	VAL	CG1	-37.21	-21.91	69.23	15.00
13	VAL	CG2	-38.14	-19.62	69.30	15.00
13	VAL	C	-36.63	-18.98	71.64	15.00
13	VAL	O	-37.62	-18.38	72.02	15.00
14	THR	N	-35.41	-18.45	71.65	15.00
14	THR	CA	-35.16	-17.08	72.07	15.00
14	THR	CB	-33.75	-16.96	72.66	15.00
14	THR	OG1	-32.79	-17.40	71.71	15.00
14	THR	CG2	-33.63	-17.80	73.91	15.00
14	THR	C	-35.32	-16.08	70.91	15.00
14	THR	O	-35.57	-16.48	69.77	15.00
15	PRO	N	-35.24	-14.77	71.20	15.00
15	PRO	CD	-35.20	-14.14	72.53	15.00
15	PRO	CA	-35.37	-13.75	70.15	15.00
15	PRO	CB	-35.25	-12.44	70.93	15.00
15	PRO	CG	-35.83	-12.79	72.26	15.00
15	PRO	C	-34.26	-13.87	69.11	15.00
15	PRO	O	-33.13	-14.23	69.44	15.00
16	VAL	N	-34.59	-13.55	67.85	15.00

TABLE II

16 VAL CA	-33.64	-13.61	66.75	15.00
16 VAL CB	-34.33	-13.31	65.40	15.00
16 VAL CG1	-33.34	-13.41	64.25	15.00
16 VAL CG2	-35.47	-14.26	65.19	15.00
16 VAL C	-32.48	-12.65	66.96	15.00
16 VAL O	-32.69	-11.49	67.32	15.00
17 LYS N	-31.28	-13.13	66.71	15.00
17 LYS CA	-30.07	-12.35	66.86	15.00
17 LYS CB	-29.12	-13.04	67.84	15.00
17 LYS CG	-29.68	-13.07	69.24	15.00
17 LYS CD	-28.91	-14.03	70.13	15.00
17 LYS CE	-29.54	-14.07	71.53	15.00
17 LYS NZ	-31.02	-14.22	71.43	15.00
17 LYS C	-29.39	-12.14	65.52	15.00
17 LYS O	-29.72	-12.79	64.54	15.00
18 ASN N	-28.42	-11.23	65.50	15.00
18 ASN CA	-27.68	-10.87	64.29	15.00
18 ASN CB	-27.77	-9.36	64.10	15.00
18 ASN CG	-27.26	-8.90	62.75	15.00
18 ASN OD1	-26.16	-9.25	62.32	15.00
18 ASN ND2	-28.07	-8.10	62.08	15.00
18 ASN C	-26.23	-11.28	64.45	15.00
18 ASN O	-25.55	-10.79	65.35	15.00
19 GLN N	-25.72	-12.16	63.60	15.00
19 GLN CA	-24.33	-12.56	63.73	15.00
19 GLN CB	-24.00	-13.81	62.90	15.00
19 GLN CG	-24.44	-13.80	61.45	15.00
19 GLN CD	-24.06	-15.09	60.72	15.00
19 GLN OE1	-24.91	-15.79	60.16	15.00
19 GLN NE2	-22.77	-15.41	60.71	15.00
19 GLN C	-23.40	-11.40	63.39	15.00
19 GLN O	-22.27	-11.33	63.88	15.00
20 GLY N	-23.91	-10.46	62.60	15.00
20 GLY CA	-23.14	-9.30	62.21	15.00
20 GLY C	-22.11	-9.67	61.16	15.00
20 GLY O	-22.39	-10.50	60.28	15.00
21 GLN N	-20.93	-9.08	61.26	15.00
21 GLN CA	-19.85	-9.33	60.32	15.00
21 GLN CB	-19.08	-8.03	60.01	15.00
21 GLN CG	-19.94	-6.78	59.84	15.00
21 GLN CD	-20.87	-6.85	58.64	15.00
21 GLN OE1	-20.43	-6.78	57.49	15.00
21 GLN NE2	-22.17	-6.95	58.90	15.00

TABLE II

21	GLN	C	-18.91	-10.35	60.98	15.00
21	GLN	O	-17.86	-10.01	61.52	15.00
22	CYS	N	-19.31	-11.61	60.97	15.00
22	CYS	CA	-18.53	-12.68	61.58	15.00
22	CYS	C	-19.27	-13.95	61.19	15.00
22	CYS	O	-20.48	-14.03	61.36	15.00
22	CYS	CB	-18.50	-12.50	63.11	15.00
22	CYS	SG	-17.85	-13.86	64.14	15.00
23	GLY	N	-18.56	-14.88	60.56	15.00
23	GLY	CA	-19.19	-16.12	60.13	15.00
23	GLY	C	-19.43	-17.05	61.30	15.00
23	GLY	O	-18.94	-18.17	61.31	15.00
24	SER	N	-20.24	-16.60	62.25	15.00
24	SER	CA	-20.56	-17.36	63.44	15.00
24	SER	CB	-20.46	-16.45	64.66	15.00
24	SER	OG	-21.23	-15.30	64.42	15.00
24	SER	C	-21.95	-17.97	63.37	15.00
24	SER	O	-22.54	-18.31	64.40	15.00
25	CYS	N	-22.49	-18.14	62.17	15.00
25	CYS	CA	-23.81	-18.74	62.02	15.00
25	CYS	CB	-24.21	-18.82	60.54	15.00
25	CYS	SG	-23.17	-19.85	59.47	15.00
25	CYS	C	-23.88	-20.12	62.68	15.00
25	CYS	O	-24.96	-20.59	63.04	15.00
25	INH	C1	-26.94	-9.70	58.69	15.00
25	INH	C2	-26.28	-10.48	59.65	15.00
25	INH	C3	-25.12	-11.19	59.30	15.00
25	INH	C4	-24.61	-11.12	58.00	15.00
25	INH	C5	-25.28	-10.33	57.05	15.00
25	INH	C6	-26.44	-9.62	57.39	15.00
25	INH	C7	-23.37	-11.90	57.62	15.00
25	INH	O8	-23.43	-13.32	57.82	15.00
25	INH	C9	-22.85	-14.36	57.02	15.00
25	INH	O10	-21.63	-14.58	56.99	15.00
25	INH	C11	-23.27	-16.14	55.41	15.00
25	INH	C12	-22.06	-15.67	54.58	15.00
25	INH	C13	-22.16	-15.18	53.14	15.00
25	INH	C14	-20.77	-15.22	52.56	15.00
25	INH	C15	-23.13	-16.04	52.32	15.00
25	INH	C16	-22.95	-17.51	56.01	15.00
25	INH	O17	-23.60	-18.50	55.66	15.00
25	INH	N18	-21.92	-17.60	56.86	15.00
25	INH	C19	-21.48	-18.89	57.42	15.00

TABLE II

25	INH C20	-20.01	-19.11	57.02	15.00
25	INH C21	-19.59	-19.34	55.56	15.00
25	INH C22	-19.45	-20.84	55.30	15.00
25	INH C23	-18.25	-18.64	55.30	15.00
25	INH N24	-23.71	-15.07	56.30	15.00
25	INH C25	-21.62	-19.06	58.94	15.00
25	INH O26	-21.55	-17.95	59.50	15.00
25	INH C27	-20.53	-20.00	59.45	15.00
25	INH O28	-20.36	-21.26	58.72	15.00
25	INH C29	-19.70	-22.40	59.29	15.00
25	INH C30	-19.53	-23.60	58.35	15.00
25	INH C31	-20.80	-24.42	58.08	15.00
26	TRP N	-22.73	-20.75	62.90	15.00
26	TRP CA	-22.65	-22.06	63.54	15.00
26	TRP CB	-21.30	-22.75	63.25	15.00
26	TRP CG	-20.09	-22.04	63.79	15.00
26	TRP CD2	-19.48	-22.23	65.08	15.00
26	TRP CE2	-18.36	-21.38	65.14	15.00
26	TRP CE3	-19.77	-23.04	66.19	15.00
26	TRP CD1	-19.33	-21.11	63.15	15.00
26	TRP NE1	-18.29	-20.70	63.95	15.00
26	TRP CZ2	-17.53	-21.31	66.27	15.00
26	TRP CZ3	-18.94	-22.97	67.31	15.00
26	TRP CH2	-17.83	-22.11	67.33	15.00
26	TRP C	-22.89	-22.02	65.06	15.00
26	TRP O	-23.59	-22.87	65.61	15.00
27	ALA N	-22.34	-21.01	65.75	15.00
27	ALA CA	-22.49	-20.86	67.19	15.00
27	ALA CB	-21.58	-19.78	67.71	15.00
27	ALA C	-23.93	-20.53	67.54	15.00
27	ALA O	-24.46	-20.98	68.55	15.00
28	PHE N	-24.55	-19.71	66.70	15.00
28	PHE CA	-25.93	-19.33	66.91	15.00
28	PHE CB	-26.33	-18.21	65.94	15.00
28	PHE CG	-25.73	-16.88	66.28	15.00
28	PHE CD1	-24.51	-16.49	65.73	15.00
28	PHE CD2	-26.34	-16.04	67.19	15.00
28	PHE CE1	-23.92	-15.30	66.11	15.00
28	PHE CE2	-25.75	-14.85	67.57	15.00
28	PHE CZ	-24.54	-14.48	67.02	15.00
28	PHE C	-26.82	-20.55	66.75	15.00
28	PHE O	-27.75	-20.75	67.51	15.00
29	SER N	-26.49	-21.39	65.78	15.00

TABLE II

29	SER CA	-27.25	-22.61	65.53	15.00
29	SER CB	-26.69	-23.33	64.31	15.00
29	SER OG	-27.48	-24.45	63.98	15.00
29	SER C	-27.16	-23.52	66.74	15.00
29	SER O	-28.17	-23.93	67.30	15.00
30	SER N	-25.92	-23.82	67.14	15.00
30	SER CA	-25.63	-24.69	68.27	15.00
30	SER CB	-24.13	-24.77	68.46	15.00
30	SER OG	-23.51	-24.96	67.22	15.00
30	SER C	-26.27	-24.16	69.55	15.00
30	SER O	-26.82	-24.92	70.35	15.00
31	VAL N	-26.17	-22.85	69.75	15.00
31	VAL CA	-26.75	-22.24	70.93	15.00
31	VAL CB	-26.25	-20.78	71.09	15.00
31	VAL CG1	-27.32	-19.87	71.63	15.00
31	VAL CG2	-25.06	-20.75	72.01	15.00
31	VAL C	-28.27	-22.35	70.84	15.00
31	VAL O	-28.94	-22.62	71.82	15.00
32	GLY N	-28.80	-22.28	69.63	15.00
32	GLY CA	-30.23	-22.39	69.44	15.00
32	GLY C	-30.80	-23.73	69.86	15.00
32	GLY O	-31.91	-23.80	70.38	15.00
33	ALA N	-30.05	-24.80	69.59	15.00
33	ALA CA	-30.46	-26.15	69.95	15.00
33	ALA CB	-29.65	-27.18	69.17	15.00
33	ALA C	-30.28	-26.35	71.44	15.00
33	ALA O	-31.16	-26.89	72.11	15.00
34	LEU N	-29.14	-25.91	71.97	15.00
34	LEU CA	-28.87	-26.01	73.40	15.00
34	LEU CB	-27.54	-25.36	73.74	15.00
34	LEU CG	-26.26	-26.09	73.37	15.00
34	LEU CD1	-25.09	-25.16	73.59	15.00
34	LEU CD2	-26.10	-27.34	74.21	15.00
34	LEU C	-29.98	-25.32	74.18	15.00
34	LEU O	-30.45	-25.85	75.18	15.00
35	GLU N	-30.43	-24.16	73.69	15.00
35	GLU CA	-31.51	-23.39	74.33	15.00
35	GLU CB	-31.65	-22.03	73.66	15.00
35	GLU CG	-30.44	-21.12	73.81	15.00
35	GLU CD	-30.54	-19.82	73.03	15.00
35	GLU OE1	-31.35	-19.71	72.09	15.00
35	GLU OE2	-29.77	-18.91	73.35	15.00
35	GLU C	-32.84	-24.12	74.28	15.00

TABLE II

35	GLU O	-33.67	-24.00	75.19	15.00
36	GLY N	-33.09	-24.86	73.21	15.00
36	GLY CA	-34.33	-25.59	73.09	15.00
36	GLY C	-34.37	-26.71	74.11	15.00
36	GLY O	-35.37	-26.91	74.80	15.00
37	GLN N	-33.26	-27.43	74.25	15.00
37	GLN CA	-33.18	-28.52	75.20	15.00
37	GLN CB	-31.92	-29.34	74.98	15.00
37	GLN CG	-31.94	-30.12	73.69	15.00
37	GLN CD	-33.17	-31.00	73.57	15.00
37	GLN OE1	-33.42	-31.85	74.43	15.00
37	GLN NE2	-33.95	-30.79	72.53	15.00
37	GLN C	-33.24	-28.01	76.63	15.00
37	GLN O	-33.97	-28.56	77.47	15.00
38	LEU N	-32.52	-26.92	76.89	15.00
38	LEU CA	-32.51	-26.31	78.21	15.00
38	LEU CB	-31.79	-24.96	78.17	15.00
38	LEU CG	-31.83	-24.13	79.46	15.00
38	LEU CD1	-31.00	-24.83	80.53	15.00
38	LEU CD2	-31.30	-22.73	79.20	15.00
38	LEU C	-33.94	-26.11	78.69	15.00
38	LEU O	-34.30	-26.51	79.79	15.00
39	LYS N	-34.77	-25.51	77.85	15.00
39	LYS CA	-36.16	-25.26	78.20	15.00
39	LYS CB	-36.85	-24.43	77.11	15.00
39	LYS CG	-38.06	-23.64	77.59	15.00
39	LYS CD	-39.32	-24.48	77.65	15.00
39	LYS CE	-40.53	-23.66	78.07	15.00
39	LYS NZ	-40.50	-23.27	79.50	15.00
39	LYS C	-36.89	-26.59	78.36	15.00
39	LYS O	-37.71	-26.75	79.25	15.00
40	LYS N	-36.57	-27.57	77.53	15.00
40	LYS CA	-37.25	-28.86	77.63	15.00
40	LYS CB	-36.85	-29.79	76.48	15.00
40	LYS CG	-37.77	-31.00	76.39	15.00
40	LYS CD	-37.48	-31.90	75.22	15.00
40	LYS CE	-38.53	-32.99	75.17	15.00
40	LYS NZ	-38.45	-33.78	73.92	15.00
40	LYS C	-36.98	-29.55	78.95	15.00
40	LYS O	-37.90	-30.11	79.56	15.00
41	LYS N	-35.74	-29.45	79.42	15.00
41	LYS CA	-35.35	-30.09	80.66	15.00
41	LYS CB	-33.87	-30.48	80.61	15.00

TABLE II

41	LYS	CG	-33.50	-31.39	79.43	15.00
41	LYS	CD	-34.48	-32.55	79.32	15.00
41	LYS	CE	-34.33	-33.33	78.02	15.00
41	LYS	NZ	-35.59	-34.07	77.73	15.00
41	LYS	C	-35.67	-29.31	81.94	15.00
41	LYS	O	-36.36	-29.82	82.81	15.00
42	THR	N	-35.20	-28.08	82.07	15.00
42	THR	CA	-35.45	-27.32	83.29	15.00
42	THR	CB	-34.31	-26.34	83.57	15.00
42	THR	OG1	-34.40	-25.23	82.67	15.00
42	THR	CG2	-32.98	-27.04	83.36	15.00
42	THR	C	-36.77	-26.54	83.35	15.00
42	THR	O	-37.19	-26.11	84.43	15.00
43	GLY	N	-37.42	-26.34	82.21	15.00
43	GLY	CA	-38.67	-25.60	82.16	15.00
43	GLY	C	-38.49	-24.09	82.05	15.00
43	GLY	O	-39.45	-23.33	81.92	15.00
44	LYS	N	-37.25	-23.62	82.11	15.00
44	LYS	CA	-36.99	-22.20	82.03	15.00
44	LYS	CB	-36.47	-21.70	83.37	15.00
44	LYS	CG	-37.07	-22.42	84.57	15.00
44	LYS	CD	-36.69	-21.78	85.90	15.00
44	LYS	CE	-35.51	-22.46	86.59	15.00
44	LYS	NZ	-35.95	-23.54	87.52	15.00
44	LYS	C	-35.98	-21.94	80.92	15.00
44	LYS	O	-34.92	-22.58	80.87	15.00
45	LEU	N	-36.32	-21.02	80.04	15.00
45	LEU	CA	-35.47	-20.64	78.90	15.00
45	LEU	CB	-36.33	-20.13	77.75	15.00
45	LEU	CG	-35.67	-19.77	76.42	15.00
45	LEU	CD1	-35.27	-21.03	75.66	15.00
45	LEU	CD2	-36.67	-18.97	75.62	15.00
45	LEU	C	-34.47	-19.58	79.29	15.00
45	LEU	O	-34.68	-18.81	80.22	15.00
46	LEU	N	-33.38	-19.50	78.54	15.00
46	LEU	CA	-32.33	-18.54	78.81	15.00
46	LEU	CB	-31.43	-19.09	79.91	15.00
46	LEU	CG	-30.45	-18.17	80.63	15.00
46	LEU	CD1	-31.17	-16.89	81.03	15.00
46	LEU	CD2	-29.91	-18.88	81.84	15.00
46	LEU	C	-31.55	-18.33	77.51	15.00
46	LEU	O	-31.62	-19.14	76.60	15.00
47	ASN	N	-30.84	-17.22	77.39	15.00

TABLE II

47 ASN CA	-30.04	-16.97	76.20	15.00
47 ASN CB	-30.04	-15.48	75.85	15.00
47 ASN CG	-31.37	-15.02	75.33	15.00
47 ASN OD1	-32.19	-14.49	76.08	15.00
47 ASN ND2	-31.59	-15.20	74.05	15.00
47 ASN C	-28.62	-17.42	76.46	15.00
47 ASN O	-27.96	-16.92	77.37	15.00
48 LEU N	-28.15	-18.40	75.69	15.00
48 LEU CA	-26.80	-18.91	75.86	15.00
48 LEU CB	-26.74	-20.39	75.53	15.00
48 LEU CG	-27.64	-21.29	76.40	15.00
48 LEU CD1	-27.37	-22.73	76.07	15.00
48 LEU CD2	-27.39	-21.05	77.86	15.00
48 LEU C	-25.79	-18.10	75.06	15.00
48 LEU O	-26.16	-17.33	74.17	15.00
49 SER N	-24.51	-18.27	75.36	15.00
49 SER CA	-23.45	-17.50	74.71	15.00
49 SER CB	-22.34	-17.20	75.73	15.00
49 SER OG	-21.21	-16.57	75.14	15.00
49 SER C	-22.81	-18.05	73.44	15.00
49 SER O	-22.00	-18.98	73.49	15.00
50 PRO N	-23.17	-17.49	72.28	15.00
50 PRO CD	-24.25	-16.53	71.99	15.00
50 PRO CA	-22.56	-17.98	71.04	15.00
50 PRO CB	-23.40	-17.29	69.95	15.00
50 PRO CG	-23.89	-16.05	70.62	15.00
50 PRO C	-21.10	-17.55	71.00	15.00
50 PRO O	-20.25	-18.21	70.41	15.00
51 GLN N	-20.79	-16.45	71.69	15.00
51 GLN CA	-19.43	-15.93	71.75	15.00
51 GLN CB	-19.40	-14.60	72.52	15.00
51 GLN CG	-18.07	-13.86	72.44	15.00
51 GLN CD	-17.86	-13.13	71.13	15.00
51 GLN OE1	-18.70	-12.34	70.70	15.00
51 GLN NE2	-16.72	-13.37	70.49	15.00
51 GLN C	-18.52	-16.94	72.44	15.00
51 GLN O	-17.43	-17.24	71.95	15.00
52 ASN N	-18.97	-17.50	73.56	15.00
52 ASN CA	-18.21	-18.49	74.31	15.00
52 ASN CB	-19.13	-19.10	75.38	15.00
52 ASN CG	-18.41	-20.00	76.37	15.00
52 ASN OD1	-18.80	-20.05	77.53	15.00
52 ASN ND2	-17.40	-20.73	75.93	15.00

TABLE II

52 ASN C	-17.77	-19.57	73.34	15.00
52 ASN O	-16.66	-20.11	73.43	15.00
53 LEU N	-18.65	-19.89	72.39	15.00
53 LEU CA	-18.37	-20.90	71.39	15.00
53 LEU CB	-19.67	-21.37	70.73	15.00
53 LEU CG	-20.66	-22.13	71.63	15.00
53 LEU CD1	-21.88	-22.54	70.82	15.00
53 LEU CD2	-20.00	-23.35	72.23	15.00
53 LEU C	-17.40	-20.39	70.35	15.00
53 LEU O	-16.45	-21.09	69.98	15.00
54 VAL N	-17.59	-19.15	69.91	15.00
54 VAL CA	-16.73	-18.54	68.89	15.00
54 VAL CB	-17.24	-17.11	68.51	15.00
54 VAL CG1	-16.31	-16.45	67.49	15.00
54 VAL CG2	-18.63	-17.19	67.92	15.00
54 VAL C	-15.27	-18.47	69.36	15.00
54 VAL O	-14.36	-18.89	68.64	15.00
55 ASP N	-15.06	-17.98	70.58	15.00
55 ASP CA	-13.73	-17.83	71.15	15.00
55 ASP CB	-13.78	-16.81	72.29	15.00
55 ASP CG	-14.32	-15.46	71.87	15.00
55 ASP OD1	-14.20	-15.10	70.68	15.00
55 ASP OD2	-14.86	-14.76	72.75	15.00
55 ASP C	-13.05	-19.09	71.70	15.00
55 ASP O	-11.81	-19.13	71.78	15.00
56 CYS N	-13.81	-20.12	72.07	15.00
56 CYS CA	-13.22	-21.32	72.67	15.00
56 CYS C	-13.29	-22.63	71.91	15.00
56 CYS O	-12.56	-23.59	72.23	15.00
56 CYS CB	-13.83	-21.53	74.05	15.00
56 CYS SG	-14.01	-20.02	75.04	15.00
57 VAL N	-14.19	-22.77	70.96	15.00
57 VAL CA	-14.26	-24.02	70.22	15.00
57 VAL CB	-15.60	-24.16	69.48	15.00
57 VAL CG1	-15.62	-25.44	68.67	15.00
57 VAL CG2	-16.73	-24.15	70.48	15.00
57 VAL C	-13.09	-24.06	69.25	15.00
57 VAL O	-13.23	-23.80	68.06	15.00
58 SER N	-11.91	-24.40	69.77	15.00
58 SER CA	-10.67	-24.46	69.00	15.00
58 SER CB	-9.53	-24.83	69.93	15.00
58 SER OG	-10.02	-25.66	70.98	15.00
58 SER C	-10.66	-25.38	67.79	15.00

TABLE II

58	SER O	-9.70	-25.38	67.02	15.00
59	GLU N	-11.70	-26.18	67.64	15.00
59	GLU CA	-11.82	-27.10	66.50	15.00
59	GLU CB	-12.70	-28.31	66.86	15.00
59	GLU CG	-12.16	-29.19	67.99	15.00
59	GLU CD	-12.31	-28.56	69.36	15.00
59	GLU OE1	-13.46	-28.38	69.83	15.00
59	GLU OE2	-11.28	-28.23	69.97	15.00
59	GLU C	-12.44	-26.34	65.33	15.00
59	GLU O	-12.44	-26.81	64.19	15.00
60	ASN N	-13.03	-25.19	65.61	15.00
60	ASN CA	-13.64	-24.37	64.58	15.00
60	ASN CB	-15.08	-23.98	64.97	15.00
60	ASN CG	-16.03	-25.16	64.95	15.00
60	ASN OD1	-17.08	-25.12	65.58	15.00
60	ASN ND2	-15.68	-26.20	64.22	15.00
60	ASN C	-12.79	-23.12	64.31	15.00
60	ASN O	-11.88	-22.80	65.06	15.00
61	ASP N	-13.13	-22.40	63.25	15.00
61	ASP CA	-12.38	-21.21	62.87	15.00
61	ASP CB	-12.30	-21.14	61.34	15.00
61	ASP CG	-10.95	-20.64	60.84	15.00
61	ASP OD1	-10.04	-20.40	61.65	15.00
61	ASP OD2	-10.80	-20.50	59.60	15.00
61	ASP C	-12.97	-19.91	63.44	15.00
61	ASP O	-12.70	-18.83	62.93	15.00
62	GLY N	-13.78	-19.99	64.49	15.00
62	GLY CA	-14.37	-18.79	65.05	15.00
62	GLY C	-15.25	-18.07	64.05	15.00
62	GLY O	-16.26	-18.59	63.58	15.00
63	CYS N	-14.89	-16.85	63.70	15.00
63	CYS CA	-15.67	-16.11	62.72	15.00
63	CYS C	-15.48	-16.70	61.33	15.00
63	CYS O	-16.15	-16.28	60.39	15.00
63	CYS CB	-15.30	-14.62	62.69	15.00
63	CYS SG	-15.85	-13.63	64.12	15.00
64	GLY N	-14.54	-17.62	61.19	15.00
64	GLY CA	-14.29	-18.25	59.90	15.00
64	GLY C	-15.24	-19.41	59.67	15.00
64	GLY O	-15.32	-19.97	58.57	15.00
65	GLY N	-15.97	-19.80	60.70	15.00
65	GLY CA	-16.91	-20.91	60.56	15.00
65	GLY C	-16.55	-22.16	61.33	15.00

TABLE II

65 GLY O	-15.46	-22.30	61.90	15.00
66 GLY N	-17.47	-23.10	61.38	15.00
66 GLY CA	-17.25	-24.34	62.07	15.00
66 GLY C	-18.51	-25.15	61.93	15.00
66 GLY O	-19.46	-24.72	61.29	15.00
67 TYR N	-18.50	-26.35	62.49	15.00
67 TYR CA	-19.66	-27.22	62.44	15.00
67 TYR CB	-19.25	-28.66	62.13	15.00
67 TYR CG	-18.41	-28.83	60.89	15.00
67 TYR CD1	-19.00	-29.00	59.64	15.00
67 TYR CE1	-18.22	-29.18	58.51	15.00
67 TYR CD2	-17.03	-28.83	60.98	15.00
67 TYR CE2	-16.25	-29.01	59.86	15.00
67 TYR CZ	-16.84	-29.18	58.63	15.00
67 TYR OH	-16.03	-29.34	57.52	15.00
67 TYR C	-20.27	-27.16	63.83	15.00
67 TYR O	-19.59	-26.85	64.80	15.00
68 MET N	-21.55	-27.48	63.93	15.00
68 MET CA	-22.24	-27.45	65.20	15.00
68 MET CB	-23.75	-27.51	65.00	15.00
68 MET CG	-24.34	-26.31	64.22	15.00
68 MET SD	-23.95	-26.25	62.46	15.00
68 MET CE	-25.40	-26.96	61.77	15.00
68 MET C	-21.76	-28.58	66.11	15.00
68 MET O	-21.49	-28.37	67.29	15.00
69 THR N	-21.57	-29.78	65.56	15.00
69 THR CA	-21.13	-30.94	66.33	15.00
69 THR CB	-20.92	-32.18	65.44	15.00
69 THR OG1	-20.10	-31.83	64.31	15.00
69 THR CG2	-22.26	-32.69	64.93	15.00
69 THR C	-19.85	-30.65	67.12	15.00
69 THR O	-19.69	-31.11	68.26	15.00
70 ASN N	-18.95	-29.84	66.55	15.00
70 ASN CA	-17.71	-29.46	67.22	15.00
70 ASN CB	-16.73	-28.81	66.24	15.00
70 ASN CG	-15.97	-29.81	65.39	15.00
70 ASN OD1	-15.41	-29.45	64.37	15.00
70 ASN ND2	-15.92	-31.06	65.83	15.00
70 ASN C	-17.96	-28.52	68.39	15.00
70 ASN O	-17.14	-28.42	69.30	15.00
71 ALA N	-19.06	-27.78	68.35	15.00
71 ALA CA	-19.42	-26.86	69.44	15.00
71 ALA CB	-20.32	-25.76	68.92	15.00

TABLE II

71 ALA C	-20.12	-27.66	70.53	15.00
71 ALA O	-19.94	-27.42	71.73	15.00
72 PHE N	-20.96	-28.60	70.13	15.00
72 PHE CA	-21.67	-29.44	71.08	15.00
72 PHE CB	-22.56	-30.44	70.34	15.00
72 PHE CG	-23.74	-29.82	69.63	15.00
72 PHE CD1	-24.33	-28.66	70.11	15.00
72 PHE CD2	-24.27	-30.43	68.50	15.00
72 PHE CE1	-25.45	-28.12	69.48	15.00
72 PHE CE2	-25.39	-29.90	67.87	15.00
72 PHE CZ	-25.98	-28.74	68.35	15.00
72 PHE C	-20.60	-30.19	71.89	15.00
72 PHE O	-20.60	-30.15	73.12	15.00
73 GLN N	-19.64	-30.81	71.21	15.00
73 GLN CA	-18.58	-31.56	71.87	15.00
73 GLN CB	-17.64	-32.18	70.82	15.00
73 GLN CG	-16.55	-33.13	71.36	15.00
73 GLN CD	-17.07	-34.54	71.69	15.00
73 GLN OE1	-17.16	-34.93	72.87	15.00
73 GLN NE2	-17.37	-35.32	70.65	15.00
73 GLN C	-17.81	-30.69	72.87	15.00
73 GLN O	-17.46	-31.13	73.96	15.00
74 TYR N	-17.55	-29.43	72.53	15.00
74 TYR CA	-16.82	-28.56	73.44	15.00
74 TYR CB	-16.43	-27.25	72.75	15.00
74 TYR CG	-16.11	-26.12	73.70	15.00
74 TYR CD1	-14.83	-25.93	74.20	15.00
74 TYR CE1	-14.54	-24.93	75.11	15.00
74 TYR CD2	-17.11	-25.25	74.14	15.00
74 TYR CE2	-16.84	-24.23	75.06	15.00
74 TYR CZ	-15.55	-24.08	75.53	15.00
74 TYR OH	-15.28	-23.08	76.45	15.00
74 TYR C	-17.62	-28.25	74.70	15.00
74 TYR O	-17.05	-28.00	75.76	15.00
75 VAL N	-18.94	-28.18	74.59	15.00
75 VAL CA	-19.77	-27.89	75.75	15.00
75 VAL CB	-21.21	-27.54	75.33	15.00
75 VAL CG1	-22.04	-27.14	76.54	15.00
75 VAL CG2	-21.20	-26.39	74.33	15.00
75 VAL C	-19.74	-29.11	76.68	15.00
75 VAL O	-19.87	-28.99	77.90	15.00
76 GLN N	-19.50	-30.29	76.09	15.00
76 GLN CA	-19.43	-31.54	76.84	15.00

TABLE II

76 GLN CB	-19.51	-32.72	75.88	15.00
76 GLN CG	-19.44	-34.10	76.53	15.00
76 GLN CD	-19.41	-35.21	75.50	15.00
76 GLN OE1	-20.45	-35.67	75.05	15.00
76 GLN NE2	-18.23	-35.64	75.12	15.00
76 GLN C	-18.15	-31.64	77.66	15.00
76 GLN O	-18.20	-31.71	78.89	15.00
77 LYS N	-17.00	-31.64	77.00	15.00
77 LYS CA	-15.72	-31.75	77.70	15.00
77 LYS CB	-14.60	-32.13	76.73	15.00
77 LYS CG	-14.72	-31.53	75.36	15.00
77 LYS CD	-13.52	-31.92	74.50	15.00
77 LYS CE	-13.77	-31.61	73.03	15.00
77 LYS NZ	-14.25	-30.21	72.83	15.00
77 LYS C	-15.29	-30.55	78.56	15.00
77 LYS O	-14.36	-30.63	79.36	15.00
78 ASN N	-15.94	-29.41	78.38	15.00
78 ASN CA	-15.62	-28.22	79.15	15.00
78 ASN CB	-15.75	-26.98	78.27	15.00
78 ASN CG	-15.54	-25.69	79.03	15.00
78 ASN OD1	-14.43	-25.40	79.46	15.00
78 ASN ND2	-16.60	-24.91	79.16	15.00
78 ASN C	-16.60	-28.14	80.32	15.00
78 ASN O	-16.47	-27.32	81.22	15.00
79 ARG N	-17.60	-29.01	80.27	15.00
79 ARG CA	-18.63	-29.08	81.29	15.00
79 ARG CB	-18.06	-29.64	82.60	15.00
79 ARG CG	-17.45	-31.04	82.42	15.00
79 ARG CD	-17.13	-31.71	83.75	15.00
79 ARG NE	-18.34	-32.20	84.40	15.00
79 ARG CZ	-18.91	-33.37	84.15	15.00
79 ARG NH1	-18.36	-34.20	83.26	15.00
79 ARG NH2	-20.05	-33.70	84.75	15.00
79 ARG C	-19.36	-27.77	81.50	15.00
79 ARG O	-19.57	-27.33	82.64	15.00
80 GLY N	-19.75	-27.14	80.39	15.00
80 GLY CA	-20.48	-25.89	80.49	15.00
80 GLY C	-20.34	-24.84	79.40	15.00
80 GLY O	-19.34	-24.78	78.67	15.00
81 ILE N	-21.39	-24.02	79.30	15.00
81 ILE CA	-21.46	-22.91	78.36	15.00
81 ILE CB	-22.22	-23.28	77.05	15.00
81 ILE CG2	-23.65	-23.63	77.33	15.00

TABLE II

81 ILE CG1	-22.16	-22.09	76.08	15.00
81 ILE CD1	-22.80	-22.35	74.75	15.00
81 ILE C	-22.15	-21.75	79.07	15.00
81 ILE O	-23.20	-21.93	79.71	15.00
82 ASP N	-21.51	-20.59	79.03	15.00
82 ASP CA	-22.01	-19.37	79.65	15.00
82 ASP CB	-20.99	-18.24	79.46	15.00
82 ASP CG	-19.78	-18.37	80.35	15.00
82 ASP OD1	-18.71	-17.88	79.95	15.00
82 ASP OD2	-19.91	-18.93	81.47	15.00
82 ASP C	-23.36	-18.86	79.13	15.00
82 ASP O	-23.86	-19.29	78.09	15.00
83 SER N	-23.91	-17.90	79.86	15.00
83 SER CA	-25.16	-17.25	79.50	15.00
83 SER CB	-25.99	-16.98	80.76	15.00
83 SER OG	-25.21	-16.38	81.78	15.00
83 SER C	-24.75	-15.93	78.85	15.00
83 SER O	-23.63	-15.45	79.05	15.00
84 GLU N	-25.64	-15.33	78.07	15.00
84 GLU CA	-25.32	-14.09	77.39	15.00
84 GLU CB	-26.48	-13.65	76.52	15.00
84 GLU CG	-26.16	-12.52	75.57	15.00
84 GLU CD	-25.34	-12.95	74.38	15.00
84 GLU OE1	-24.85	-14.10	74.35	15.00
84 GLU OE2	-25.19	-12.13	73.45	15.00
84 GLU C	-24.88	-12.96	78.31	15.00
84 GLU O	-24.03	-12.14	77.94	15.00
85 ASP N	-25.44	-12.87	79.52	15.00
85 ASP CA	-25.03	-11.81	80.45	15.00
85 ASP CB	-25.92	-11.77	81.71	15.00
85 ASP CG	-25.48	-10.69	82.73	15.00
85 ASP OD1	-24.60	-9.85	82.41	15.00
85 ASP OD2	-26.00	-10.66	83.87	15.00
85 ASP C	-23.59	-12.02	80.86	15.00
85 ASP O	-22.83	-11.07	81.00	15.00
86 ALA N	-23.18	-13.27	81.05	15.00
86 ALA CA	-21.82	-13.56	81.47	15.00
86 ALA CB	-21.76	-14.91	82.14	15.00
86 ALA C	-20.78	-13.48	80.36	15.00
86 ALA O	-19.62	-13.15	80.59	15.00
87 TYR N	-21.18	-13.74	79.12	15.00
87 TYR CA	-20.23	-13.71	78.02	15.00
87 TYR CB	-19.79	-15.15	77.74	15.00

TABLE II

87 TYR CG	-18.44	-15.33	77.08	15.00
87 TYR CD1	-17.91	-14.37	76.21	15.00
87 TYR CE1	-16.69	-14.59	75.57	15.00
87 TYR CD2	-17.72	-16.51	77.28	15.00
87 TYR CE2	-16.50	-16.73	76.64	15.00
87 TYR CZ	-16.00	-15.77	75.79	15.00
87 TYR OH	-14.79	-16.02	75.16	15.00
87 TYR C	-20.92	-13.13	76.79	15.00
87 TYR O	-21.26	-13.88	75.86	15.00
88 PRO N	-21.19	-11.80	76.79	15.00
88 PRO CD	-21.02	-10.93	77.96	15.00
88 PRO CA	-21.85	-11.07	75.70	15.00
88 PRO CB	-21.91	-9.64	76.23	15.00
88 PRO CG	-22.06	-9.86	77.72	15.00
88 PRO C	-21.13	-11.13	74.36	15.00
88 PRO O	-19.90	-11.11	74.31	15.00
89 TYR N	-21.93	-11.18	73.31	15.00
89 TYR CA	-21.47	-11.28	71.92	15.00
89 TYR CB	-22.64	-11.80	71.09	15.00
89 TYR CG	-22.28	-12.14	69.68	15.00
89 TYR CD1	-21.43	-13.20	69.39	15.00
89 TYR CE1	-21.07	-13.48	68.09	15.00
89 TYR CD2	-22.75	-11.36	68.63	15.00
89 TYR CE2	-22.39	-11.63	67.32	15.00
89 TYR CZ	-21.55	-12.69	67.06	15.00
89 TYR OH	-21.15	-12.93	65.77	15.00
89 TYR C	-20.94	-9.96	71.34	15.00
89 TYR O	-21.71	-9.04	71.08	15.00
90 VAL N	-19.64	-9.86	71.12	15.00
90 VAL CA	-19.06	-8.63	70.58	15.00
90 VAL CB	-17.75	-8.27	71.27	15.00
90 VAL CG1	-17.98	-8.12	72.76	15.00
90 VAL CG2	-16.69	-9.32	70.99	15.00
90 VAL C	-18.87	-8.65	69.07	15.00
90 VAL O	-18.28	-7.74	68.50	15.00
91 GLY N	-19.30	-9.73	68.44	15.00
91 GLY CA	-19.20	-9.84	67.00	15.00
91 GLY C	-17.86	-10.11	66.36	15.00
91 GLY O	-17.67	-9.84	65.18	15.00
92 GLN N	-16.91	-10.66	67.11	15.00
92 GLN CA	-15.59	-10.97	66.57	15.00
92 GLN CB	-14.80	-9.69	66.32	15.00
92 GLN CG	-14.73	-8.76	67.51	15.00

TABLE II

92 GLN CD	-13.95	-7.50	67.19	15.00
92 GLN OE1	-12.73	-7.54	67.06	15.00
92 GLN NE2	-14.65	-6.38	67.02	15.00
92 GLN C	-14.83	-11.87	67.53	15.00
92 GLN O	-15.17	-11.94	68.71	15.00
93 GLU N	-13.80	-12.53	67.04	15.00
93 GLU CA	-13.02	-13.45	67.85	15.00
93 GLU CB	-12.36	-14.52	66.98	15.00
93 GLU CG	-11.54	-13.97	65.80	15.00
93 GLU CD	-11.57	-14.90	64.59	15.00
93 GLU OE1	-10.51	-15.16	63.98	15.00
93 GLU OE2	-12.67	-15.36	64.22	15.00
93 GLU C	-11.99	-12.78	68.74	15.00
93 GLU O	-11.29	-11.86	68.33	15.00
94 GLU N	-11.89	-13.29	69.97	15.00
94 GLU CA	-10.96	-12.78	70.96	15.00
94 GLU CB	-11.65	-11.74	71.84	15.00
94 GLU CG	-12.68	-12.34	72.79	15.00
94 GLU CD	-13.96	-11.54	72.88	15.00
94 GLU OE1	-13.96	-10.36	72.44	15.00
94 GLU OE2	-14.97	-12.08	73.38	15.00
94 GLU C	-10.54	-13.98	71.82	15.00
94 GLU O	-10.95	-15.10	71.55	15.00
95 SER N	-9.72	-13.74	72.84	15.00
95 SER CA	-9.26	-14.80	73.73	15.00
95 SER CB	-8.26	-14.23	74.75	15.00
95 SER OG	-7.14	-13.65	74.09	15.00
95 SER C	-10.41	-15.51	74.46	15.00
95 SER O	-11.34	-14.87	74.95	15.00
96 CYS N	-10.37	-16.84	74.53	15.00
96 CYS CA	-11.44	-17.57	75.21	15.00
96 CYS C	-11.55	-17.03	76.62	15.00
96 CYS O	-10.58	-17.04	77.37	15.00
96 CYS CB	-11.13	-19.06	75.26	15.00
96 CYS SG	-12.35	-20.02	76.20	15.00
97 MET N	-12.72	-16.51	76.97	15.00
97 MET CA	-12.95	-15.95	78.31	15.00
97 MET CB	-13.50	-14.53	78.21	15.00
97 MET CG	-12.65	-13.51	77.52	15.00
97 MET SD	-13.49	-11.94	77.83	15.00
97 MET CE	-14.95	-12.05	76.75	15.00
97 MET C	-13.95	-16.74	79.15	15.00
97 MET O	-14.60	-16.15	80.02	15.00

TABLE II

98 TYR N	-14.08	-18.05	78.94	15.00
98 TYR CA	-15.05	-18.82	79.70	15.00
98 TYR CB	-14.89	-20.33	79.47	15.00
98 TYR CG	-15.95	-21.14	80.19	15.00
98 TYR CD1	-17.30	-21.01	79.88	15.00
98 TYR CE1	-18.28	-21.71	80.58	15.00
98 TYR CD2	-15.61	-22.00	81.23	15.00
98 TYR CE2	-16.58	-22.70	81.94	15.00
98 TYR CZ	-17.91	-22.55	81.62	15.00
98 TYR OH	-18.86	-23.22	82.33	15.00
98 TYR C	-14.99	-18.51	81.20	15.00
98 TYR O	-13.92	-18.32	81.77	15.00
99 ASN N	-16.16	-18.49	81.82	15.00
99 ASN CA	-16.30	-18.18	83.23	15.00
99 ASN CB	-16.73	-16.72	83.37	15.00
99 ASN CG	-17.06	-16.32	84.81	15.00
99 ASN OD1	-16.96	-17.13	85.74	15.00
99 ASN ND2	-17.47	-15.06	84.98	15.00
99 ASN C	-17.34	-19.10	83.86	15.00
99 ASN O	-18.55	-18.87	83.72	15.00
100 PRO N	-16.89	-20.13	84.60	15.00
100 PRO CD	-15.46	-20.39	84.86	15.00
100 PRO CA	-17.73	-21.12	85.29	15.00
100 PRO CB	-16.74	-21.80	86.22	15.00
100 PRO CG	-15.49	-21.81	85.41	15.00
100 PRO C	-18.84	-20.46	86.07	15.00
100 PRO O	-19.93	-21.02	86.20	15.00
101 THR N	-18.58	-19.26	86.58	15.00
101 THR CA	-19.58	-18.53	87.34	15.00
101 THR CB	-18.99	-17.20	87.84	15.00
101 THR OG1	-17.76	-17.48	88.53	15.00
101 THR CG2	-19.95	-16.50	88.80	15.00
101 THR C	-20.78	-18.25	86.46	15.00
101 THR O	-21.93	-18.29	86.93	15.00
102 GLY N	-20.52	-17.99	85.18	15.00
102 GLY CA	-21.57	-17.69	84.23	15.00
102 GLY C	-22.29	-18.89	83.62	15.00
102 GLY O	-23.36	-18.73	83.04	15.00
103 LYS N	-21.70	-20.07	83.72	15.00
103 LYS CA	-22.30	-21.29	83.17	15.00
103 LYS CB	-21.60	-22.52	83.76	15.00
103 LYS CG	-22.34	-23.84	83.55	15.00
103 LYS CD	-21.59	-24.99	84.23	15.00

TABLE II

103 LYS CE	-22.56	-26.02	84.79	15.00
103 LYS NZ	-23.48	-26.58	83.76	15.00
103 LYS C	-23.81	-21.37	83.41	15.00
103 LYS O	-24.27	-21.24	84.54	15.00
104 ALA N	-24.58	-21.60	82.35	15.00
104 ALA CA	-26.04	-21.70	82.45	15.00
104 ALA CB	-26.69	-20.52	81.78	15.00
104 ALA C	-26.60	-22.99	81.88	15.00
104 ALA O	-27.76	-23.32	82.12	15.00
105 ALA N	-25.81	-23.71	81.09	15.00
105 ALA CA	-26.26	-24.97	80.50	15.00
105 ALA CB	-26.99	-24.72	79.19	15.00
105 ALA C	-25.10	-25.92	80.28	15.00
105 ALA O	-23.93	-25.52	80.38	15.00
106 LYS N	-25.41	-27.18	79.98	15.00
106 LYS CA	-24.40	-28.19	79.72	15.00
106 LYS CB	-23.77	-28.66	81.03	15.00
106 LYS CG	-24.73	-29.25	82.04	15.00
106 LYS CD	-24.01	-29.56	83.33	15.00
106 LYS CE	-22.75	-30.37	83.07	15.00
106 LYS NZ	-23.05	-31.63	82.31	15.00
106 LYS C	-25.06	-29.34	78.99	15.00
106 LYS O	-26.28	-29.39	78.94	15.00
107 CYS N	-24.27	-30.21	78.38	15.00
107 CYS CA	-24.83	-31.36	77.65	15.00
107 CYS CB	-25.14	-30.97	76.20	15.00
107 CYS SG	-23.71	-31.01	75.11	15.00
107 CYS C	-23.95	-32.61	77.67	15.00
107 CYS O	-22.73	-32.53	77.81	15.00
108 ARG N	-24.59	-33.76	77.53	15.00
108 ARG CA	-23.92	-35.05	77.54	15.00
108 ARG CB	-24.66	-36.03	78.46	15.00
108 ARG CG	-26.18	-35.81	78.55	15.00
108 ARG CD	-26.93	-37.01	79.17	15.00
108 ARG NE	-27.06	-38.15	78.25	15.00
108 ARG CZ	-28.19	-38.49	77.62	15.00
108 ARG NH1	-29.31	-37.79	77.80	15.00
108 ARG NH2	-28.22	-39.56	76.84	15.00
108 ARG C	-23.70	-35.67	76.15	15.00
108 ARG O	-23.77	-36.88	75.98	15.00
109 GLY N	-23.44	-34.83	75.16	15.00
109 GLY CA	-23.19	-35.32	73.82	15.00
109 GLY C	-24.08	-34.73	72.75	15.00

TABLE II

109	GLY O	-24.72	-33.69	72.94	15.00
110	TYR N	-24.15	-35.41	71.61	15.00
110	TYR CA	-24.97	-34.95	70.50	15.00
110	TYR CB	-24.19	-33.91	69.71	15.00
110	TYR CG	-22.97	-34.46	68.99	15.00
110	TYR CD1	-21.71	-34.43	69.59	15.00
110	TYR CE1	-20.59	-34.90	68.91	15.00
110	TYR CD2	-23.07	-34.99	67.71	15.00
110	TYR CE2	-21.97	-35.45	67.03	15.00
110	TYR CZ	-20.73	-35.40	67.63	15.00
110	TYR OH	-19.63	-35.82	66.93	15.00
110	TYR C	-25.31	-36.11	69.57	15.00
110	TYR O	-24.61	-37.12	69.54	15.00
111	ARG N	-26.35	-35.94	68.76	15.00
111	ARG CA	-26.74	-36.97	67.82	15.00
111	ARG CB	-28.02	-37.68	68.29	15.00
111	ARG CG	-27.87	-38.44	69.61	15.00
111	ARG CD	-29.17	-39.16	70.00	15.00
111	ARG NE	-29.49	-40.25	69.07	15.00
111	ARG CZ	-28.84	-41.41	69.03	15.00
111	ARG NH1	-29.20	-42.34	68.14	15.00
111	ARG NH2	-27.85	-41.65	69.88	15.00
111	ARG C	-27.00	-36.34	66.45	15.00
111	ARG O	-27.71	-35.34	66.34	15.00
112	GLU N	-26.39	-36.90	65.42	15.00
112	GLU CA	-26.57	-36.42	64.06	15.00
112	GLU CB	-25.27	-36.56	63.27	15.00
112	GLU CG	-24.17	-35.62	63.74	15.00
112	GLU CD	-22.80	-35.91	63.12	15.00
112	GLU OE1	-22.22	-34.99	62.47	15.00
112	GLU OE2	-22.29	-37.05	63.30	15.00
112	GLU C	-27.68	-37.26	63.45	15.00
112	GLU O	-27.84	-38.43	63.80	15.00
113	ILE N	-28.50	-36.63	62.61	15.00
113	ILE CA	-29.60	-37.28	61.90	15.00
113	ILE CB	-30.69	-36.23	61.48	15.00
113	ILE CG2	-31.45	-36.68	60.25	15.00
113	ILE CG1	-31.68	-35.99	62.62	15.00
113	ILE CD1	-31.14	-35.16	63.73	15.00
113	ILE C	-29.00	-37.94	60.66	15.00
113	ILE O	-28.03	-37.44	60.10	15.00
114	PRO N	-29.54	-39.09	60.23	15.00
114	PRO CD	-30.62	-39.89	60.83	15.00

TABLE II

114 PRO CA	-29.00	-39.75	59.04	15.00
114 PRO CB	-30.00	-40.89	58.81	15.00
114 PRO CG	-30.41	-41.24	60.19	15.00
114 PRO C	-28.97	-38.80	57.86	15.00
114 PRO O	-29.98	-38.20	57.52	15.00
115 GLU N	-27.80	-38.73	57.22	15.00
115 GLU CA	-27.56	-37.86	56.07	15.00
115 GLU CB	-26.14	-38.07	55.52	15.00
115 GLU CG	-25.92	-37.52	54.10	15.00
115 GLU CD	-24.48	-37.06	53.82	15.00
115 GLU OE1	-23.52	-37.73	54.28	15.00
115 GLU OE2	-24.30	-36.02	53.15	15.00
115 GLU C	-28.55	-38.00	54.93	15.00
115 GLU O	-28.57	-39.02	54.26	15.00
116 GLY N	-29.31	-36.94	54.69	15.00
116 GLY CA	-30.27	-36.94	53.60	15.00
116 GLY C	-31.66	-37.41	53.97	15.00
116 GLY O	-32.57	-37.40	53.14	15.00
117 ASN N	-31.86	-37.78	55.24	15.00
117 ASN CA	-33.15	-38.29	55.69	15.00
117 ASN CB	-32.94	-39.38	56.73	15.00
117 ASN CG	-34.19	-40.18	56.99	15.00
117 ASN OD1	-35.32	-39.68	56.89	15.00
117 ASN ND2	-34.00	-41.46	57.33	15.00
117 ASN C	-34.07	-37.22	56.27	15.00
117 ASN O	-33.93	-36.82	57.43	15.00
118 GLU N	-35.06	-36.79	55.50	15.00
118 GLU CA	-35.97	-35.78	55.99	15.00
118 GLU CB	-36.70	-35.07	54.85	15.00
118 GLU CG	-36.04	-33.77	54.42	15.00
118 GLU CD	-36.91	-32.99	53.45	15.00
118 GLU OE1	-36.81	-33.22	52.23	15.00
118 GLU OE2	-37.72	-32.15	53.91	15.00
118 GLU C	-36.97	-36.33	56.98	15.00
118 GLU O	-37.46	-35.59	57.83	15.00
119 LYS N	-37.32	-37.61	56.90	15.00
119 LYS CA	-38.27	-38.14	57.87	15.00
119 LYS CB	-38.85	-39.49	57.42	15.00
119 LYS CG	-40.19	-39.34	56.68	15.00
119 LYS CD	-40.08	-38.40	55.47	15.00
119 LYS CE	-41.47	-38.06	54.90	15.00
119 LYS NZ	-42.26	-37.19	55.83	15.00
119 LYS C	-37.62	-38.24	59.24	15.00

TABLE II

119	LYS O	-38.23	-37.90	60.26	15.00
120	ALA N	-36.35	-38.62	59.28	15.00
120	ALA CA	-35.63	-38.70	60.54	15.00
120	ALA CB	-34.25	-39.25	60.33	15.00
120	ALA C	-35.55	-37.30	61.16	15.00
120	ALA O	-35.58	-37.15	62.38	15.00
121	LEU N	-35.45	-36.27	60.32	15.00
121	LEU CA	-35.38	-34.89	60.82	15.00
121	LEU CB	-34.93	-33.91	59.73	15.00
121	LEU CG	-34.80	-32.45	60.19	15.00
121	LEU CD1	-33.77	-32.34	61.30	15.00
121	LEU CD2	-34.42	-31.56	59.03	15.00
121	LEU C	-36.74	-34.48	61.36	15.00
121	LEU O	-36.83	-33.80	62.38	15.00
122	LYS N	-37.79	-34.89	60.66	15.00
122	LYS CA	-39.16	-34.58	61.05	15.00
122	LYS CB	-40.14	-35.19	60.07	15.00
122	LYS CG	-41.57	-34.80	60.31	15.00
122	LYS CD	-42.49	-35.45	59.32	15.00
122	LYS CE	-43.95	-35.16	59.67	15.00
122	LYS NZ	-44.88	-35.66	58.60	15.00
122	LYS C	-39.41	-35.15	62.44	15.00
122	LYS O	-39.87	-34.44	63.33	15.00
123	ARG N	-39.12	-36.44	62.62	15.00
123	ARG CA	-39.29	-37.10	63.90	15.00
123	ARG CB	-38.84	-38.58	63.84	15.00
123	ARG CG	-39.74	-39.50	62.99	15.00
123	ARG CD	-39.33	-40.97	63.13	15.00
123	ARG NE	-37.95	-41.22	62.73	15.00
123	ARG CZ	-37.42	-42.43	62.51	15.00
123	ARG NH1	-38.15	-43.53	62.66	15.00
123	ARG NH2	-36.17	-42.53	62.08	15.00
123	ARG C	-38.46	-36.37	64.94	15.00
123	ARG O	-39.01	-35.82	65.89	15.00
124	ALA N	-37.15	-36.31	64.71	15.00
124	ALA CA	-36.22	-35.65	65.62	15.00
124	ALA CB	-34.86	-35.50	64.98	15.00
124	ALA C	-36.70	-34.29	66.11	15.00
124	ALA O	-36.67	-34.02	67.31	15.00
125	VAL N	-37.16	-33.45	65.19	15.00
125	VAL CA	-37.66	-32.13	65.55	15.00
125	VAL CB	-38.00	-31.28	64.27	15.00
125	VAL CG1	-38.50	-29.89	64.64	15.00

TABLE II

125 VAL CG2	-36.77	-31.11	63.41	15.00
125 VAL C	-38.87	-32.25	66.47	15.00
125 VAL O	-39.03	-31.46	67.41	15.00
126 ALA N	-39.71	-33.26	66.28	15.00
126 ALA CA	-40.90	-33.44	67.11	15.00
126 ALA CB	-42.00	-34.13	66.32	15.00
126 ALA C	-40.64	-34.18	68.44	15.00
126 ALA O	-41.32	-33.93	69.44	15.00
127 ARG N	-39.67	-35.09	68.46	15.00
127 ARG CA	-39.36	-35.83	69.68	15.00
127 ARG CB	-38.79	-37.22	69.36	15.00
127 ARG CG	-39.80	-38.34	69.36	15.00
127 ARG CD	-40.24	-38.71	67.96	15.00
127 ARG NE	-39.78	-40.04	67.58	15.00
127 ARG CZ	-40.46	-40.88	66.80	15.00
127 ARG NH1	-39.94	-42.06	66.52	15.00
127 ARG NH2	-41.66	-40.57	66.33	15.00
127 ARG C	-38.36	-35.09	70.56	15.00
127 ARG O	-38.41	-35.20	71.78	15.00
128 VAL N	-37.44	-34.37	69.94	15.00
128 VAL CA	-36.42	-33.64	70.68	15.00
128 VAL CB	-35.07	-33.78	69.99	15.00
128 VAL CG1	-33.97	-33.24	70.88	15.00
128 VAL CG2	-34.81	-35.23	69.64	15.00
128 VAL C	-36.75	-32.17	70.84	15.00
128 VAL O	-36.91	-31.68	71.94	15.00
129 GLY N	-36.85	-31.47	69.72	15.00
129 GLY CA	-37.13	-30.05	69.75	15.00
129 GLY C	-36.29	-29.43	68.64	15.00
129 GLY O	-35.92	-30.14	67.70	15.00
130 PRO N	-35.92	-28.15	68.76	15.00
130 PRO CD	-36.24	-27.22	69.86	15.00
130 PRO CA	-35.11	-27.49	67.75	15.00
130 PRO CB	-34.80	-26.14	68.39	15.00
130 PRO CG	-36.01	-25.88	69.20	15.00
130 PRO C	-33.83	-28.24	67.40	15.00
130 PRO O	-33.02	-28.57	68.28	15.00
131 VAL N	-33.63	-28.47	66.11	15.00
131 VAL CA	-32.46	-29.17	65.62	15.00
131 VAL CB	-32.89	-30.36	64.73	15.00
131 VAL CG1	-31.68	-31.12	64.19	15.00
131 VAL CG2	-33.78	-31.29	65.53	15.00
131 VAL C	-31.59	-28.20	64.81	15.00

TABLE II

131 VAL O	-32.10	-27.31	64.12	15.00
132 SER N	-30.28	-28.33	64.94	15.00
132 SER CA	-29.35	-27.48	64.21	15.00
132 SER CB	-28.02	-27.41	64.95	15.00
132 SER OG	-28.18	-26.80	66.21	15.00
132 SER C	-29.16	-28.09	62.83	15.00
132 SER O	-28.84	-29.27	62.71	15.00
133 VAL N	-29.37	-27.32	61.78	15.00
133 VAL CA	-29.21	-27.82	60.42	15.00
133 VAL CB	-30.58	-28.02	59.71	15.00
133 VAL CG1	-31.50	-28.91	60.54	15.00
133 VAL CG2	-31.24	-26.68	59.44	15.00
133 VAL C	-28.37	-26.84	59.60	15.00
133 VAL O	-28.20	-25.68	59.99	15.00
134 ALA N	-27.82	-27.30	58.48	15.00
134 ALA CA	-27.00	-26.45	57.62	15.00
134 ALA CB	-25.58	-26.95	57.57	15.00
134 ALA C	-27.65	-26.50	56.26	15.00
134 ALA O	-28.14	-27.55	55.86	15.00
135 ILE N	-27.66	-25.38	55.55	15.00
135 ILE CA	-28.30	-25.28	54.23	15.00
135 ILE CB	-29.70	-24.57	54.29	15.00
135 ILE CG2	-30.71	-25.39	55.10	15.00
135 ILE CG1	-29.54	-23.15	54.87	15.00
135 ILE CD1	-30.81	-22.34	54.88	15.00
135 ILE C	-27.46	-24.44	53.29	15.00
135 ILE O	-26.40	-23.92	53.66	15.00
136 ASP N	-27.97	-24.32	52.07	15.00
136 ASP CA	-27.34	-23.50	51.04	15.00
136 ASP CB	-27.56	-24.11	49.65	15.00
136 ASP CG	-27.02	-23.23	48.53	15.00
136 ASP OD1	-27.80	-22.84	47.64	15.00
136 ASP OD2	-25.83	-22.91	48.54	15.00
136 ASP C	-28.06	-22.16	51.14	15.00
136 ASP O	-29.21	-22.03	50.74	15.00
137 ALA N	-27.43	-21.17	51.76	15.00
137 ALA CA	-28.07	-19.87	51.86	15.00
137 ALA CB	-27.97	-19.34	53.26	15.00
137 ALA C	-27.47	-18.89	50.85	15.00
137 ALA O	-27.92	-17.75	50.72	15.00
138 SER N	-26.43	-19.33	50.15	15.00
138 SER CA	-25.79	-18.51	49.14	15.00
138 SER CB	-24.36	-19.00	48.90	15.00

TABLE II

138 SER OG	-23.55	-18.75	50.04	15.00
138 SER C	-26.61	-18.61	47.87	15.00
138 SER O	-26.41	-19.53	47.07	15.00
139 LEU N	-27.56	-17.70	47.74	15.00
139 LEU CA	-28.46	-17.66	46.60	15.00
139 LEU CB	-29.32	-18.92	46.55	15.00
139 LEU CG	-30.03	-19.30	45.25	15.00
139 LEU CD1	-29.04	-19.96	44.31	15.00
139 LEU CD2	-31.14	-20.28	45.54	15.00
139 LEU C	-29.35	-16.43	46.82	15.00
139 LEU O	-29.99	-16.29	47.87	15.00
140 THR N	-29.39	-15.54	45.83	15.00
140 THR CA	-30.17	-14.30	45.90	15.00
140 THR CB	-30.15	-13.57	44.52	15.00
140 THR OG1	-29.95	-14.53	45.47	15.00
140 THR CG2	-29.05	-12.52	44.48	15.00
140 THR C	-31.60	-14.43	46.41	15.00
140 THR O	-32.02	-13.70	47.31	15.00
141 SER N	-32.35	-15.38	45.88	15.00
141 SER CA	-33.74	-15.58	46.27	15.00
141 SER CB	-34.42	-16.62	45.36	15.00
141 SER OG	-33.62	-17.78	45.21	15.00
141 SER C	-33.92	-15.96	47.74	15.00
141 SER O	-34.99	-15.74	48.33	15.00
142 PHE N	-32.90	-16.52	48.37	15.00
142 PHE CA	-33.01	-16.91	49.77	15.00
142 PHE CB	-31.92	-17.91	50.15	15.00
142 PHE CG	-31.91	-18.26	51.61	15.00
142 PHE CD1	-32.74	-19.26	52.10	15.00
142 PHE CD2	-31.09	-17.58	52.50	15.00
142 PHE CE1	-32.74	-19.58	53.45	15.00
142 PHE CE2	-31.09	-17.90	53.87	15.00
142 PHE CZ	-31.92	-18.89	54.34	15.00
142 PHE C	-32.87	-15.67	50.62	15.00
142 PHE O	-33.64	-15.45	51.55	15.00
143 GLN N	-31.90	-14.85	50.24	15.00
143 GLN CA	-31.58	-13.63	50.96	15.00
143 GLN CB	-30.25	-13.12	50.48	15.00
143 GLN CG	-29.21	-14.20	50.55	15.00
143 GLN CD	-27.89	-13.73	50.06	15.00
143 GLN OE1	-27.33	-12.78	50.59	15.00
143 GLN NE2	-27.36	-14.40	49.05	15.00
143 GLN C	-32.63	-12.53	50.92	15.00

TABLE II

143	GLN	O	-32.79	-11.82	51.91	15.00
144	PHE	N	-33.31	-12.35	49.79	15.00
144	PHE	CA	-34.36	-11.32	49.70	15.00
144	PHE	CB	-34.28	-10.50	48.39	15.00
144	PHE	CG	-34.49	-11.30	47.11	15.00
144	PHE	CD1	-33.53	-11.26	46.11	15.00
144	PHE	CD2	-35.66	-12.02	46.88	15.00
144	PHE	CE1	-33.74	-11.93	44.90	15.00
144	PHE	CE2	-35.88	-12.69	45.67	15.00
144	PHE	CZ	-34.91	-12.64	44.68	15.00
144	PHE	C	-35.77	-11.88	49.96	15.00
144	PHE	O	-36.77	-11.36	49.45	15.00
145	TYR	N	-35.82	-12.95	50.76	15.00
145	TYR	CA	-37.05	-13.64	51.13	15.00
145	TYR	CB	-36.69	-14.96	51.83	15.00
145	TYR	CG	-37.83	-15.59	52.60	15.00
145	TYR	CD1	-38.64	-16.56	52.01	15.00
145	TYR	CE1	-39.71	-17.11	52.70	15.00
145	TYR	CD2	-38.11	-15.20	53.91	15.00
145	TYR	CE2	-39.18	-15.74	54.60	15.00
145	TYR	CZ	-39.98	-16.69	53.99	15.00
145	TYR	OH	-41.05	-17.22	54.66	15.00
145	TYR	C	-37.79	-12.74	52.10	15.00
145	TYR	O	-37.16	-12.04	52.89	15.00
146	SER	N	-39.12	-12.80	52.09	15.00
146	SER	CA	-39.93	-11.97	52.99	15.00
146	SER	CB	-40.22	-10.61	52.35	15.00
146	SER	OG	-40.75	-10.75	51.05	15.00
146	SER	C	-41.25	-12.62	53.43	15.00
146	SER	O	-41.83	-12.21	54.43	15.00
147	LYS	N	-41.74	-13.59	52.66	15.00
147	LYS	CA	-42.98	-14.28	52.99	15.00
147	LYS	CB	-44.19	-13.35	52.82	15.00
147	LYS	CG	-44.40	-12.86	51.40	15.00
147	LYS	CD	-45.58	-11.90	51.31	15.00
147	LYS	CE	-46.86	-12.63	50.95	15.00
147	LYS	NZ	-48.03	-11.69	50.96	15.00
147	LYS	C	-43.18	-15.52	52.13	15.00
147	LYS	O	-42.61	-15.62	51.04	15.00
148	GLY	N	-44.00	-16.45	52.62	15.00
148	GLY	CA	-44.27	-17.68	51.88	15.00
148	GLY	C	-43.30	-18.81	52.16	15.00
148	GLY	O	-42.38	-18.69	52.97	15.00

TABLE II

149 VAL N	-43.52	-19.94	51.51	15.00
149 VAL CA	-42.66	-21.10	51.68	15.00
149 VAL CB	-43.47	-22.41	51.46	15.00
149 VAL CG1	-42.59	-23.63	51.61	15.00
149 VAL CG2	-44.62	-22.47	52.45	15.00
149 VAL C	-41.57	-20.96	50.62	15.00
149 VAL O	-41.84	-20.56	49.50	15.00
150 TYR N	-40.34	-21.30	50.96	15.00
150 TYR CA	-39.24	-21.14	50.02	15.00
150 TYR CB	-38.02	-20.54	50.73	15.00
150 TYR CG	-36.80	-20.39	49.85	15.00
150 TYR CD1	-36.77	-19.48	48.80	15.00
150 TYR CE1	-35.66	-19.36	47.97	15.00
150 TYR CD2	-35.67	-21.18	50.05	15.00
150 TYR CE2	-34.56	-21.07	49.24	15.00
150 TYR CZ	-34.56	-20.16	48.20	15.00
150 TYR OH	-33.45	-20.04	47.40	15.00
150 TYR C	-38.83	-22.39	49.27	15.00
150 TYR O	-38.66	-23.45	49.85	15.00
151 TYR N	-38.62	-22.22	47.97	15.00
151 TYR CA	-38.17	-23.31	47.12	15.00
151 TYR CB	-39.33	-24.21	46.71	15.00
151 TYR CG	-38.86	-25.44	45.98	15.00
151 TYR CD1	-37.95	-26.30	46.56	15.00
151 TYR CE1	-37.46	-27.40	45.87	15.00
151 TYR CD2	-39.29	-25.71	44.68	15.00
151 TYR CE2	-38.81	-26.81	43.98	15.00
151 TYR CZ	-37.89	-27.65	44.58	15.00
151 TYR OH	-37.37	-28.73	43.90	15.00
151 TYR C	-37.49	-22.74	45.88	15.00
151 TYR O	-37.97	-21.79	45.28	15.00
152 ASP N	-36.36	-23.32	45.49	15.00
152 ASP CA	-35.64	-22.85	44.31	15.00
152 ASP CB	-34.72	-21.69	44.66	15.00
152 ASP CG	-34.07	-21.09	43.44	15.00
152 ASP OD1	-33.12	-21.69	42.92	15.00
152 ASP OD2	-34.52	-20.01	43.01	15.00
152 ASP C	-34.83	-23.96	43.66	15.00
152 ASP O	-33.85	-24.45	44.23	15.00
153 GLU N	-35.21	-24.32	42.44	15.00
153 GLU CA	-34.53	-25.36	41.69	15.00
153 GLU CB	-34.98	-25.36	40.21	15.00
153 GLU CG	-35.22	-23.98	39.55	15.00

TABLE II

153 GLU CD	-33.95	-23.34	38.93	15.00
153 GLU OE1	-33.38	-22.41	39.56	15.00
153 GLU OE2	-33.56	-23.73	37.80	15.00
153 GLU C	-33.02	-25.27	41.80	15.00
153 GLU O	-32.36	-26.29	42.00	15.00
154 SER N	-32.48	-24.05	41.74	15.00
154 SER CA	-31.02	-23.84	41.81	15.00
154 SER CB	-30.65	-22.45	41.31	15.00
154 SER OG	-30.66	-22.41	39.90	15.00
154 SER C	-30.37	-24.06	43.16	15.00
154 SER O	-29.14	-23.91	43.30	15.00
155 CYS N	-31.15	-24.39	44.19	15.00
155 CYS CA	-30.56	-24.61	45.49	15.00
155 CYS C	-29.70	-25.86	45.37	15.00
155 CYS O	-30.17	-26.88	44.86	15.00
155 CYS CB	-31.63	-24.79	46.55	15.00
155 CYS SG	-31.06	-24.07	48.11	15.00
156 ASN N	-28.43	-25.75	45.74	15.00
156 ASN CA	-27.50	-26.87	45.66	15.00
156 ASN CB	-26.13	-26.39	45.18	15.00
156 ASN CG	-25.14	-27.52	44.97	15.00
156 ASN OD1	-25.51	-28.70	44.95	15.00
156 ASN ND2	-23.88	-27.16	44.80	15.00
156 ASN C	-27.34	-27.66	46.95	15.00
156 ASN O	-26.57	-27.31	47.85	15.00
157 SER N	-28.03	-28.79	46.98	15.00
157 SER CA	-28.03	-29.71	48.10	15.00
157 SER CB	-28.72	-31.00	47.65	15.00
157 SER OG	-29.25	-30.85	46.33	15.00
157 SER C	-26.63	-30.03	48.63	15.00
157 SER O	-26.46	-30.47	49.77	15.00
158 ASP N	-25.61	-29.83	47.80	15.00
158 ASP CA	-24.23	-30.12	48.18	15.00
158 ASP CB	-23.50	-30.73	47.00	15.00
158 ASP CG	-23.99	-32.13	46.66	15.00
158 ASP OD1	-24.82	-32.27	45.74	15.00
158 ASP OD2	-23.57	-33.09	47.34	15.00
158 ASP C	-23.44	-28.95	48.72	15.00
158 ASP O	-22.48	-29.13	49.48	15.00
159 ASN N	-23.80	-27.73	48.33	15.00
159 ASN CA	-23.05	-26.56	48.81	15.00
159 ASN CB	-23.07	-25.44	47.75	15.00
159 ASN CG	-22.15	-24.26	48.11	15.00

TABLE II

159 ASN OD1	-22.30	-23.64	49.16	15.00
159 ASN ND2	-21.21	-23.95	47.22	15.00
159 ASN C	-23.63	-26.08	50.13	15.00
159 ASN O	-24.43	-25.14	50.17	15.00
160 LEU N	-23.27	-26.74	51.23	15.00
160 LEU CA	-23.78	-26.33	52.55	15.00
160 LEU CB	-23.76	-27.50	53.53	15.00
160 LEU CG	-24.57	-28.73	53.10	15.00
160 LEU CD1	-24.08	-29.96	53.84	15.00
160 LEU CD2	-26.06	-28.51	53.32	15.00
160 LEU C	-22.87	-25.21	53.02	15.00
160 LEU O	-21.70	-25.45	53.29	15.00
161 ASN N	-23.41	-24.01	53.16	15.00
161 ASN CA	-22.59	-22.86	53.54	15.00
161 ASN CB	-22.43	-21.97	52.31	15.00
161 ASN CG	-23.75	-21.64	51.67	15.00
161 ASN OD1	-24.51	-20.79	52.17	15.00
161 ASN ND2	-24.09	-22.36	50.62	15.00
161 ASN C	-23.07	-22.00	54.70	15.00
161 ASN O	-22.32	-21.20	55.27	15.00
162 HIS N	-24.34	-22.10	55.06	15.00
162 HIS CA	-24.87	-21.31	56.16	15.00
162 HIS CB	-25.90	-20.34	55.60	15.00
162 HIS CG	-26.42	-19.36	56.60	15.00
162 HIS CD2	-27.67	-19.00	56.94	15.00
162 HIS ND1	-25.58	-18.61	57.40	15.00
162 HIS CE1	-26.30	-17.82	58.18	15.00
162 HIS NE2	-27.57	-18.05	57.92	15.00
162 HIS C	-25.52	-22.24	57.17	15.00
162 HIS O	-26.26	-23.14	56.80	15.00
163 ALA N	-25.22	-22.02	58.45	15.00
163 ALA CA	-25.79	-22.84	59.53	15.00
163 ALA CB	-24.77	-23.10	60.61	15.00
163 ALA C	-27.00	-22.13	60.10	15.00
163 ALA O	-26.93	-20.95	60.48	15.00
164 VAL N	-28.10	-22.85	60.20	15.00
164 VAL CA	-29.34	-22.30	60.70	15.00
164 VAL CB	-30.25	-22.02	59.52	15.00
164 VAL CG1	-31.04	-23.26	59.13	15.00
164 VAL CG2	-31.11	-20.83	59.80	15.00
164 VAL C	-29.96	-23.25	61.73	15.00
164 VAL O	-29.32	-24.21	62.14	15.00
165 LEU N	-31.20	-22.99	62.16	15.00

TABLE II

165 LEU CA	-31.87	-23.83	63.17	15.00
165 LEU CB	-31.87	-23.10	64.52	15.00
165 LEU CG	-32.48	-23.78	65.74	15.00
165 LEU CD1	-31.58	-24.90	66.23	15.00
165 LEU CD2	-32.71	-22.77	66.84	15.00
165 LEU C	-33.31	-24.16	62.81	15.00
165 LEU O	-34.08	-23.27	62.49	15.00
166 ALA N	-33.69	-25.43	62.90	15.00
166 ALA CA	-35.06	-25.86	62.59	15.00
166 ALA CB	-35.05	-27.27	62.00	15.00
166 ALA C	-35.91	-25.81	63.86	15.00
166 ALA O	-35.69	-26.57	64.80	15.00
167 VAL N	-36.89	-24.92	63.85	15.00
167 VAL CA	-37.78	-24.65	65.00	15.00
167 VAL CB	-37.89	-23.09	65.18	15.00
167 VAL CG1	-38.97	-22.71	66.15	15.00
167 VAL CG2	-36.58	-22.55	65.68	15.00
167 VAL C	-39.16	-25.32	64.93	15.00
167 VAL O	-39.98	-25.21	65.84	15.00
168 GLY N	-39.43	-26.06	63.87	15.00
168 GLY CA	-40.71	-26.72	63.75	15.00
168 GLY C	-40.98	-27.09	62.31	15.00
168 GLY O	-40.05	-27.10	61.49	15.00
169 TYR N	-42.23	-27.39	61.99	15.00
169 TYR CA	-42.65	-27.76	60.65	15.00
169 TYR CB	-42.15	-29.17	60.29	15.00
169 TYR CG	-42.64	-30.27	61.22	15.00
169 TYR CD1	-44.00	-30.58	61.31	15.00
169 TYR CE1	-44.46	-31.57	62.15	15.00
169 TYR CD2	-41.75	-30.99	62.01	15.00
169 TYR CE2	-42.20	-31.99	62.85	15.00
169 TYR CZ	-43.56	-32.28	62.91	15.00
169 TYR OH	-44.04	-33.28	63.71	15.00
169 TYR C	-44.16	-27.70	60.54	15.00
169 TYR O	-44.85	-27.38	61.52	15.00
170 GLY N	-44.70	-28.04	59.38	15.00
170 GLY CA	-46.13	-28.00	59.18	15.00
170 GLY C	-46.49	-27.76	57.73	15.00
170 GLY O	-45.83	-28.26	56.83	15.00
171 ILE N	-47.48	-26.92	57.48	15.00
171 ILE CA	-47.95	-26.63	56.13	15.00
171 ILE CB	-49.03	-27.66	55.72	15.00
171 ILE CG2	-50.01	-27.09	54.71	15.00

TABLE II

171	ILE	CG1	-48.36	-28.95	55.21	15.00
171	ILE	CD1	-49.35	-30.05	54.82	15.00
171	ILE	C	-48.54	-25.23	56.14	15.00
171	ILE	O	-48.91	-24.71	57.20	15.00
172	GLN	N	-48.58	-24.55	55.00	15.00
172	GLN	CA	-49.16	-23.20	54.97	15.00
172	GLN	CB	-48.08	-22.18	54.62	15.00
172	GLN	CG	-48.58	-20.75	54.57	15.00
172	GLN	CD	-47.50	-19.79	54.12	15.00
172	GLN	OE1	-46.95	-19.93	53.02	15.00
172	GLN	NE2	-47.18	-18.82	54.96	15.00
172	GLN	C	-50.29	-23.15	53.96	15.00
172	GLN	O	-51.45	-22.89	54.32	15.00
173	LYS	N	-49.96	-23.36	52.68	15.00
173	LYS	CA	-50.96	-23.38	51.61	15.00
173	LYS	CB	-50.84	-22.14	50.69	15.00
173	LYS	CG	-51.09	-20.78	51.36	15.00
173	LYS	CD	-52.40	-20.72	52.16	15.00
173	LYS	CE	-53.63	-20.91	51.29	15.00
173	LYS	NZ	-54.88	-20.56	52.06	15.00
173	LYS	C	-50.66	-24.63	50.81	15.00
173	LYS	O	-50.20	-24.57	49.67	15.00
174	GLY	N	-50.86	-25.77	51.45	15.00
174	GLY	CA	-50.60	-27.04	50.79	15.00
174	GLY	C	-49.13	-27.39	50.91	15.00
174	GLY	O	-48.77	-28.52	51.28	15.00
175	ASN	N	-48.26	-26.42	50.63	15.00
175	ASN	CA	-46.83	-26.66	50.70	15.00
175	ASN	CB	-46.06	-25.48	50.10	15.00
175	ASN	CG	-46.31	-25.33	48.61	15.00
175	ASN	OD1	-47.34	-24.79	48.20	15.00
175	ASN	ND2	-45.38	-25.81	47.80	15.00
175	ASN	C	-46.33	-26.96	52.11	15.00
175	ASN	O	-46.55	-26.18	53.05	15.00
176	LYS	N	-45.69	-28.13	52.25	15.00
176	LYS	CA	-45.13	-28.55	53.53	15.00
176	LYS	CB	-44.68	-30.01	53.48	15.00
176	LYS	CG	-45.77	-31.03	53.17	15.00
176	LYS	CD	-45.27	-32.45	53.44	15.00
176	LYS	CE	-46.19	-33.50	52.85	15.00
176	LYS	NZ	-46.03	-33.64	51.36	15.00
176	LYS	C	-43.92	-27.66	53.74	15.00
176	LYS	O	-43.25	-27.27	52.77	15.00

TABLE II

177 HIS N	-43.57	-27.37	54.99	15.00
177 HIS CA	-42.44	-26.49	55.22	15.00
177 HIS CB	-42.90	-25.04	55.10	15.00
177 HIS CG	-43.81	-24.59	56.20	15.00
177 HIS CD2	-43.59	-24.40	57.52	15.00
177 HIS ND1	-45.13	-24.24	55.98	15.00
177 HIS CE1	-45.67	-23.85	57.12	15.00
177 HIS NE2	-44.76	-23.93	58.07	15.00
177 HIS C	-41.73	-26.66	56.55	15.00
177 HIS O	-42.31	-27.17	57.50	15.00
178 TRP N	-40.48	-26.20	56.61	15.00
178 TRP CA	-39.68	-26.25	57.82	15.00
178 TRP CB	-38.26	-26.73	57.52	15.00
178 TRP CG	-38.13	-28.11	57.02	15.00
178 TRP CD2	-38.29	-29.32	57.78	15.00
178 TRP CE2	-37.96	-30.39	56.93	15.00
178 TRP CE3	-38.68	-29.59	59.10	15.00
178 TRP CD1	-37.74	-28.49	55.78	15.00
178 TRP NE1	-37.62	-29.86	55.72	15.00
178 TRP CZ2	-38.00	-31.71	57.35	15.00
178 TRP CZ3	-38.72	-30.91	59.52	15.00
178 TRP CH2	-38.38	-31.96	58.64	15.00
178 TRP C	-39.60	-24.81	58.34	15.00
178 TRP O	-39.21	-23.90	57.60	15.00
179 ILE N	-39.96	-24.57	59.59	15.00
179 ILE CA	-39.89	-23.23	60.17	15.00
179 ILE CB	-40.79	-23.11	61.41	15.00
179 ILE CG2	-40.66	-21.74	62.03	15.00
179 ILE CG1	-42.24	-23.42	61.02	15.00
179 ILE CD1	-43.21	-23.40	62.15	15.00
179 ILE C	-38.44	-23.00	60.58	15.00
179 ILE O	-37.97	-23.57	61.56	15.00
180 ILE N	-37.72	-22.17	59.81	15.00
180 ILE CA	-36.31	-21.89	60.07	15.00
180 ILE CB	-35.49	-21.93	58.76	15.00
180 ILE CG2	-34.04	-21.77	59.05	15.00
180 ILE CG1	-35.73	-23.25	58.02	15.00
180 ILE CD1	-35.30	-24.46	58.78	15.00
180 ILE C	-36.03	-20.55	60.77	15.00
180 ILE O	-36.62	-19.52	60.42	15.00
181 LYS N	-35.13	-20.57	61.74	15.00
181 LYS CA	-34.73	-19.40	62.50	15.00
181 LYS CB	-34.63	-19.75	63.99	15.00

TABLE II

181 LYS CG	-34.15	-18.60	64.87	15.00
181 LYS CD	-33.79	-19.04	66.29	15.00
181 LYS CE	-33.65	-17.84	67.19	15.00
181 LYS NZ	-33.21	-18.18	68.57	15.00
181 LYS C	-33.36	-19.00	62.01	15.00
181 LYS O	-32.43	-19.79	62.05	15.00
182 ASN N	-33.20	-17.77	61.53	15.00
182 ASN CA	-31.90	-17.34	61.04	15.00
182 ASN CB	-32.07	-16.64	59.69	15.00
182 ASN CG	-30.84	-16.74	58.82	15.00
182 ASN OD1	-29.75	-17.06	59.30	15.00
182 ASN ND2	-31.01	-16.50	57.53	15.00
182 ASN C	-31.22	-16.43	62.06	15.00
182 ASN O	-31.77	-16.14	63.11	15.00
183 SER N	-30.00	-15.98	61.77	15.00
183 SER CA	-29.29	-15.10	62.69	15.00
183 SER CB	-28.07	-15.81	63.25	15.00
183 SER OG	-27.40	-16.52	62.23	15.00
183 SER C	-28.87	-13.82	61.98	15.00
183 SER O	-27.82	-13.25	62.27	15.00
184 TRP N	-29.70	-13.35	61.06	15.00
184 TRP CA	-29.40	-12.13	60.34	15.00
184 TRP CB	-29.58	-12.36	58.83	15.00
184 TRP CG	-28.57	-13.29	58.22	15.00
184 TRP CD2	-28.61	-13.87	56.90	15.00
184 TRP CE2	-27.40	-14.58	56.72	15.00
184 TRP CE3	-29.54	-13.84	55.86	15.00
184 TRP CD1	-27.39	-13.69	58.76	15.00
184 TRP NE1	-26.68	-14.46	57.87	15.00
184 TRP CZ2	-27.11	-15.26	55.53	15.00
184 TRP CZ3	-29.25	-14.52	54.67	15.00
184 TRP CH2	-28.04	-15.22	54.52	15.00
184 TRP C	-30.28	-10.98	60.82	15.00
184 TRP O	-30.61	-10.09	60.04	15.00
185 GLY N	-30.70	-11.02	62.09	15.00
185 GLY CA	-31.53	-9.96	62.66	15.00
185 GLY C	-33.03	-10.14	62.46	15.00
185 GLY O	-33.46	-10.99	61.69	15.00
186 GLU N	-33.84	-9.34	63.17	15.00
186 GLU CA	-35.30	-9.44	63.04	15.00
186 GLU CB	-36.00	-8.71	64.19	15.00
186 GLU CG	-35.52	-9.13	65.56	15.00
186 GLU CD	-36.52	-8.85	66.68	15.00

TABLE II

186	GLU	OE1	-36.30	-9.38	67.80	15.00
186	GLU	OE2	-37.51	-8.13	66.46	15.00
186	GLU	C	-35.74	-8.83	61.73	15.00
186	GLU	O	-36.83	-9.11	61.22	15.00
187	ASN	N	-34.89	-7.97	61.19	15.00
187	ASN	CA	-35.15	-7.28	59.95	15.00
187	ASN	CB	-34.04	-6.25	59.73	15.00
187	ASN	CG	-34.56	-4.94	59.17	15.00
187	ASN	OD1	-33.77	-4.07	58.80	15.00
187	ASN	ND2	-35.88	-4.76	59.16	15.00
187	ASN	C	-35.21	-8.22	58.75	15.00
187	ASN	O	-36.04	-8.04	57.86	15.00
188	TRP	N	-34.33	-9.22	58.73	15.00
188	TRP	CA	-34.26	-10.18	57.64	15.00
188	TRP	CB	-33.03	-11.07	57.79	15.00
188	TRP	CG	-32.85	-12.02	56.65	15.00
188	TRP	CD2	-33.28	-13.38	56.57	15.00
188	TRP	CE2	-32.98	-13.85	55.28	15.00
188	TRP	CE3	-33.90	-14.26	57.48	15.00
188	TRP	CD1	-32.31	-11.72	55.44	15.00
188	TRP	NE1	-32.39	-12.81	54.61	15.00
188	TRP	CZ2	-33.27	-15.15	54.86	15.00
188	TRP	CZ3	-34.20	-15.55	57.06	15.00
188	TRP	CH2	-33.88	-15.98	55.77	15.00
188	TRP	C	-35.50	-11.05	57.53	15.00
188	TRP	O	-36.10	-11.42	58.55	15.00
189	GLY	N	-35.85	-11.42	56.31	15.00
189	GLY	CA	-37.00	-12.26	56.07	15.00
189	GLY	C	-38.21	-11.92	56.90	15.00
189	GLY	O	-38.47	-10.76	57.23	15.00
190	ASN	N	-38.97	-12.94	57.27	15.00
190	ASN	CA	-40.16	-12.73	58.07	15.00
190	ASN	CB	-41.17	-13.86	57.83	15.00
190	ASN	CG	-42.55	-13.53	58.36	15.00
190	ASN	OD1	-42.70	-12.88	59.39	15.00
190	ASN	ND2	-43.57	-13.99	57.65	15.00
190	ASN	C	-39.79	-12.67	59.54	15.00
190	ASN	O	-39.85	-13.66	60.25	15.00
191	LYS	N	-39.32	-11.52	60.00	15.00
191	LYS	CA	-38.95	-11.34	61.39	15.00
191	LYS	CB	-40.19	-11.48	62.29	15.00
191	LYS	CG	-40.95	-10.18	62.44	15.00
191	LYS	CD	-42.19	-10.32	63.30	15.00

TABLE II

191 LYS CE	-43.32	-10.98	62.52	15.00
191 LYS NZ	-43.71	-10.21	61.31	15.00
191 LYS C	-37.84	-12.24	61.88	15.00
191 LYS O	-37.77	-12.55	63.06	15.00
192 GLY N	-36.94	-12.61	60.98	15.00
192 GLY CA	-35.83	-13.46	61.35	15.00
192 GLY C	-36.05	-14.91	60.98	15.00
192 GLY O	-35.12	-15.70	60.99	15.00
193 TYR N	-37.29	-15.27	60.65	15.00
193 TYR CA	-37.60	-16.64	60.28	15.00
193 TYR CB	-38.84	-17.13	61.05	15.00
193 TYR CG	-38.60	-17.31	62.52	15.00
193 TYR CD1	-38.73	-16.25	63.41	15.00
193 TYR CE1	-38.46	-16.41	64.76	15.00
193 TYR CD2	-38.19	-18.55	63.03	15.00
193 TYR CE2	-37.92	-18.71	64.38	15.00
193 TYR CZ	-38.05	-17.64	65.23	15.00
193 TYR OH	-37.77	-17.80	66.56	15.00
193 TYR C	-37.83	-16.81	58.79	15.00
193 TYR O	-38.02	-15.82	58.08	15.00
194 ILE N	-37.82	-18.06	58.35	15.00
194 ILE CA	-38.04	-18.41	56.95	15.00
194 ILE CB	-36.75	-18.32	56.10	15.00
194 ILE CG2	-35.64	-19.14	56.72	15.00
194 ILE CG1	-37.03	-18.83	54.69	15.00
194 ILE CD1	-35.86	-18.72	53.75	15.00
194 ILE C	-38.61	-19.81	56.83	15.00
194 ILE O	-38.11	-20.74	57.43	15.00
195 LEU N	-39.72	-19.92	56.10	15.00
195 LEU CA	-40.38	-21.19	55.85	15.00
195 LEU CB	-41.88	-20.96	55.65	15.00
195 LEU CG	-42.82	-20.84	56.86	15.00
195 LEU CD1	-42.19	-20.08	58.01	15.00
195 LEU CD2	-44.12	-20.18	56.42	15.00
195 LEU C	-39.76	-21.78	54.59	15.00
195 LEU O	-39.79	-21.16	53.53	15.00
196 MET N	-39.11	-22.93	54.71	15.00
196 MET CA	-38.46	-23.57	53.57	15.00
196 MET CB	-37.03	-23.97	53.96	15.00
196 MET CG	-36.09	-22.77	54.14	15.00
196 MET SD	-34.43	-23.18	54.74	15.00
196 MET CE	-33.67	-23.82	53.22	15.00
196 MET C	-39.28	-24.78	53.11	15.00

TABLE II

196 MET O	-40.09	-25.31	53.86	15.00
197 ALA N	-39.08	-25.23	51.87	15.00
197 ALA CA	-39.83	-26.37	51.32	15.00
197 ALA CB	-39.62	-26.47	49.82	15.00
197 ALA C	-39.52	-27.71	51.98	15.00
197 ALA O	-38.37	-28.15	51.98	15.00
198 ARG N	-40.56	-28.39	52.46	15.00
198 ARG CA	-40.40	-29.68	53.11	15.00
198 ARG CB	-41.17	-29.72	54.44	15.00
198 ARG CG	-41.15	-31.07	55.15	15.00
198 ARG CD	-41.43	-30.95	56.63	15.00
198 ARG NE	-42.81	-30.59	56.92	15.00
198 ARG CZ	-43.79	-31.47	57.10	15.00
198 ARG NH1	-43.54	-32.78	57.01	15.00
198 ARG NH2	-45.01	-31.05	57.42	15.00
198 ARG C	-40.82	-30.85	52.23	15.00
198 ARG O	-41.86	-30.80	51.57	15.00
199 ASN N	-40.00	-31.89	52.23	15.00
199 ASN CA	-40.25	-33.10	51.45	15.00
199 ASN CB	-41.59	-33.75	51.83	15.00
199 ASN CG	-41.57	-34.40	53.22	15.00
199 ASN OD1	-42.60	-34.43	53.91	15.00
199 ASN ND2	-40.42	-34.91	53.63	15.00
199 ASN C	-40.15	-32.94	49.94	15.00
199 ASN O	-40.49	-33.86	49.19	15.00
200 LYS N	-39.67	-31.77	49.49	15.00
200 LYS CA	-39.50	-31.55	48.05	15.00
200 LYS CB	-39.77	-30.09	47.65	15.00
200 LYS CG	-41.23	-29.79	47.39	15.00
200 LYS CD	-41.42	-28.49	46.63	15.00
200 LYS CE	-42.88	-28.03	46.65	15.00
200 LYS NZ	-43.06	-26.68	46.03	15.00
200 LYS C	-38.09	-31.95	47.69	15.00
200 LYS O	-37.28	-31.12	47.26	15.00
201 ASN N	-37.80	-33.22	47.95	15.00
201 ASN CA	-36.50	-33.81	47.65	15.00
201 ASN CB	-36.24	-33.83	46.13	15.00
201 ASN CG	-37.32	-34.57	45.35	15.00
201 ASN OD1	-37.09	-35.68	44.87	15.00
201 ASN ND2	-38.46	-33.92	45.15	15.00
201 ASN C	-35.31	-33.16	48.37	15.00
201 ASN O	-34.31	-32.84	47.74	15.00
202 ASN N	-35.43	-32.90	49.67	15.00

TABLE II

202 ASN CA	-34.32	-32.33	50.44	15.00
202 ASN CB	-33.19	-33.35	50.50	15.00
202 ASN CG	-32.27	-33.14	51.68	15.00
202 ASN OD1	-32.71	-32.70	52.75	15.00
202 ASN ND2	-31.00	-33.48	51.51	15.00
202 ASN C	-33.81	-30.99	49.89	15.00
202 ASN O	-32.60	-30.77	49.75	15.00
203 ALA N	-34.73	-30.09	49.59	15.00
203 ALA H	-35.63	-30.29	49.94	15.00
203 ALA CA	-34.40	-28.79	49.02	15.00
203 ALA CB	-35.62	-27.88	48.98	15.00
203 ALA C	-33.35	-28.09	49.90	15.00
203 ALA O	-33.51	-27.93	51.10	15.00
204 CYS N	-32.27	-27.66	49.25	15.00
204 CYS CA	-31.18	-26.94	49.91	15.00
204 CYS C	-30.38	-27.79	50.89	15.00
204 CYS O	-29.60	-27.25	51.68	15.00
204 CYS CB	-31.71	-25.68	50.59	15.00
204 CYS SG	-32.51	-24.48	49.47	15.00
205 GLY N	-30.56	-29.10	50.84	15.00
205 GLY CA	-29.83	-30.00	51.71	15.00
205 GLY C	-30.11	-29.81	53.19	15.00
205 GLY O	-29.22	-29.98	54.02	15.00
206 ILE N	-31.35	-29.51	53.52	15.00
206 ILE CA	-31.77	-29.30	54.89	15.00
206 ILE CB	-33.30	-29.10	54.96	15.00
206 ILE CG2	-34.02	-30.31	54.38	15.00
206 ILE CG1	-33.76	-28.86	56.41	15.00
206 ILE CD1	-33.48	-27.47	56.92	15.00
206 ILE C	-31.35	-30.45	55.82	15.00
206 ILE O	-30.94	-30.23	56.97	15.00
207 ALA N	-31.36	-31.68	55.31	15.00
207 ALA CA	-31.00	-32.84	56.11	15.00
207 ALA CB	-32.05	-33.93	55.95	15.00
207 ALA C	-29.61	-33.42	55.88	15.00
207 ALA O	-29.35	-34.57	56.24	15.00
208 ASN N	-28.68	-32.65	55.31	15.00
208 ASN CA	-27.33	-33.15	55.05	15.00
208 ASN CB	-26.76	-32.53	53.77	15.00
208 ASN CG	-27.34	-33.15	52.51	15.00
208 ASN OD1	-28.21	-34.02	52.57	15.00
208 ASN ND2	-26.89	-32.67	51.36	15.00
208 ASN C	-26.32	-32.95	56.20	15.00

TABLE II

208	ASN	O	-25.17	-33.40	56.12	15.00
209	LEU	N	-26.72	-32.25	57.25	15.00
209	LEU	CA	-25.84	-32.03	58.40	15.00
209	LEU	CB	-24.76	-31.00	58.04	15.00
209	LEU	CG	-23.41	-30.99	58.78	15.00
209	LEU	CD1	-22.72	-32.35	58.64	15.00
209	LEU	CD2	-22.51	-29.86	58.24	15.00
209	LEU	C	-26.67	-31.60	59.63	15.00
209	LEU	O	-26.38	-30.59	60.28	15.00
210	ALA	N	-27.72	-32.37	59.95	15.00
210	ALA	H	-28.03	-32.90	59.19	15.00
210	ALA	CA	-28.61	-32.05	61.06	15.00
210	ALA	CB	-30.02	-32.57	60.81	15.00
210	ALA	C	-28.10	-32.73	62.34	15.00
210	ALA	O	-27.62	-33.86	62.34	15.00
211	SER	N	-28.18	-32.02	63.47	15.00
211	SER	CA	-27.75	-32.59	64.74	15.00
211	SER	CB	-26.24	-32.46	64.92	15.00
211	SER	OG	-25.84	-31.12	65.06	15.00
211	SER	C	-28.45	-31.88	65.88	15.00
211	SER	O	-29.03	-30.80	65.71	15.00
212	PHE	N	-28.50	-32.51	67.04	15.00
212	PHE	CA	-29.11	-31.91	68.21	15.00
212	PHE	CB	-30.59	-32.31	68.33	15.00
212	PHE	CG	-30.81	-33.79	68.43	15.00
212	PHE	CD1	-31.11	-34.54	67.30	15.00
212	PHE	CD2	-30.72	-34.44	69.66	15.00
212	PHE	CE1	-31.32	-35.91	67.39	15.00
212	PHE	CE2	-30.92	-35.81	69.77	15.00
212	PHE	CZ	-31.23	-36.55	68.63	15.00
212	PHE	C	-28.30	-32.39	69.40	15.00
212	PHE	O	-27.66	-33.43	69.32	15.00
213	PRO	N	-28.24	-31.58	70.46	15.00
213	PRO	CD	-28.77	-30.21	70.54	15.00
213	PRO	CA	-27.48	-31.92	71.67	15.00
213	PRO	CB	-27.21	-30.55	72.28	15.00
213	PRO	CG	-28.47	-29.82	71.97	15.00
213	PRO	C	-28.27	-32.81	72.64	15.00
213	PRO	O	-29.50	-32.76	72.69	15.00
214	LYS	N	-27.57	-33.62	73.42	15.00
214	LYS	CA	-28.23	-34.49	74.37	15.00
214	LYS	CB	-27.67	-35.90	74.28	15.00
214	LYS	CG	-28.06	-36.64	73.02	15.00

TABLE II

214	LYS	CD	-27.66	-38.11	73.07	15.00
214	LYS	CE	-26.16	-38.29	73.05	15.00
214	LYS	NZ	-25.79	-39.70	72.73	15.00
214	LYS	C	-28.03	-33.95	75.77	15.00
214	LYS	O	-26.90	-33.70	76.18	15.00
215	MET	N	-29.12	-33.69	76.47	15.00
215	MET	CA	-29.06	-33.18	77.83	15.00
215	MET	CB	-29.71	-31.80	77.93	15.00
215	MET	CG	-28.74	-30.64	77.75	15.00
215	MET	SD	-29.45	-29.00	78.06	15.00
215	MET	CE	-30.38	-29.32	79.56	15.00
215	MET	C	-29.72	-34.16	78.81	15.00
215	MET	OT1	-30.39	-35.12	78.35	15.00
215	MET	OT2	-29.55	-33.97	80.04	15.00
216	HOH	OH2	-28.46	-18.77	85.58	15.00
217	HOH	OH2	-24.63	-33.99	81.97	15.00
218	HOH	OH2	-31.11	-15.95	65.82	15.00
219	HOH	OH2	-30.23	-19.59	64.13	15.00
220	HOH	OH2	-8.58	-7.31	62.36	15.00
221	HOH	OH2	-6.71	-10.79	69.96	15.00
222	HOH	OH2	-34.27	-22.79	70.48	15.00
223	HOH	OH2	-16.88	-33.68	66.52	15.00
224	HOH	OH2	-15.68	-8.93	63.11	15.00
225	HOH	OH2	-24.93	-30.84	62.42	15.00
226	HOH	OH2	-7.02	-8.27	72.29	15.00
227	HOH	OH2	-13.39	-20.80	66.92	15.00
228	HOH	OH2	-44.55	-30.12	50.27	15.00
229	HOH	OH2	-44.14	-35.34	56.06	15.00
230	HOH	OH2	-37.95	-16.02	68.44	15.00
231	HOH	OH2	-36.41	-36.82	52.05	15.00
232	HOH	OH2	-20.00	-36.75	62.15	15.00
233	HOH	OH2	-30.13	-19.30	67.02	15.00
234	HOH	OH2	-28.16	-19.22	62.41	15.00
235	HOH	OH2	-22.03	-29.95	62.71	15.00
236	HOH	OH2	-25.92	-8.85	75.85	15.00
237	HOH	OH2	-41.00	-28.78	81.30	15.00
238	HOH	OH2	-32.73	-23.15	83.59	15.00
239	HOH	OH2	-40.55	-13.35	49.90	15.00
240	HOH	OH2	-35.40	-24.36	49.00	15.00
241	HOH	OH2	-48.40	-32.54	58.07	15.00
242	HOH	OH2	-27.39	-6.75	59.53	15.00
243	HOH	OH2	-41.50	-14.46	65.52	15.00
244	HOH	OH2	-22.40	-5.47	61.33	15.00

TABLE II

245	HOH	OH2	-33.17	-27.91	70.80	15.00
246	HOH	OH2	-45.87	-26.25	75.72	15.00
247	HOH	OH2	-12.64	-13.96	81.39	15.00
248	HOH	OH2	-3.78	-18.92	74.98	15.00
249	HOH	OH2	-8.03	-17.70	78.42	15.00
250	HOH	OH2	-27.41	-34.98	59.22	15.00
251	HOH	OH2	-34.88	-10.94	53.71	15.00
252	HOH	OH2	-32.92	-27.68	46.17	15.00
253	HOH	OH2	-39.35	-16.01	44.28	15.00
254	HOH	OH2	-41.38	-34.64	56.30	15.00
255	HOH	OH2	-44.42	-18.35	73.08	15.00
256	HOH	OH2	-32.35	-13.73	61.23	15.00
257	HOH	OH2	-39.40	-8.90	59.13	15.00
258	HOH	OH2	-28.41	-8.93	68.65	15.00
259	HOH	OH2	-31.58	-6.53	63.69	15.00
260	HOH	OH2	-19.27	-8.48	63.41	15.00
261	HOH	OH2	-33.33	-20.29	70.52	15.00
262	HOH	OH2	-13.49	-22.80	78.17	15.00
263	HOH	OH2	-8.72	-18.49	72.60	15.00
264	HOH	OH2	-10.39	-28.70	76.32	15.00
265	HOH	OH2	-20.24	-31.77	61.63	15.00
266	HOH	OH2	-24.78	-46.10	72.19	15.00
267	HOH	OH2	-13.26	-33.12	68.94	15.00
268	HOH	OH2	-12.60	-26.87	72.01	15.00
269	HOH	OH2	-17.76	-34.32	80.14	15.00
270	HOH	OH2	-22.51	-37.80	70.83	15.00
271	HOH	OH2	-7.33	-12.89	66.95	15.00
272	HOH	OH2	-9.75	-17.21	68.77	15.00
273	HOH	OH2	-30.86	-20.40	48.59	15.00
274	HOH	OH2	-25.79	-24.78	42.10	15.00
275	HOH	OH2	-33.50	-37.21	50.03	15.00
276	HOH	OH2	-23.21	-24.90	43.38	15.00
277	HOH	OH2	-37.83	-31.49	44.10	15.00
278	HOH	OH2	-37.02	-30.78	51.01	15.00

TABLE III

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for the cathepsin K complex with inhibitor bis-(cbz-leuciny1)-1,3-diamino-propan-2-one.

Residue Atom	X	Y	Z	B
1 ALA CB	-54.29	-33.17	65.94	15.00
1 ALA C	-53.88	-32.69	63.50	15.00
1 ALA O	-53.42	-33.61	62.80	15.00
1 ALA N	-55.60	-34.28	64.17	15.00
1 ALA CA	-54.93	-33.01	64.57	15.00
2 PRO N	-53.52	-31.40	63.32	15.00
2 PRO CD	-53.99	-30.23	64.09	15.00
2 PRO CA	-52.52	-30.98	62.32	15.00
2 PRO CB	-52.49	-29.46	62.49	15.00
2 PRO CG	-52.83	-29.26	63.94	15.00
2 PRO C	-51.13	-31.59	62.52	15.00
2 PRO O	-50.62	-31.64	63.64	15.00
3 ASP N	-50.53	-32.08	61.44	15.00
3 ASP CA	-49.19	-32.65	61.51	15.00
3 ASP CB	-48.89	-33.49	60.27	15.00
3 ASP CG	-49.53	-34.88	60.32	15.00
3 ASP OD1	-49.43	-35.55	61.39	15.00
3 ASP OD2	-50.12	-35.29	59.28	15.00
3 ASP C	-48.24	-31.46	61.55	15.00
3 ASP O	-47.60	-31.14	60.54	15.00
4 SER N	-48.16	-30.78	62.68	15.00
4 SER CA	-47.29	-29.62	62.80	15.00
4 SER CB	-47.99	-28.35	62.27	15.00
4 SER OG	-48.14	-28.37	60.86	15.00
4 SER C	-46.84	-29.35	64.23	15.00
4 SER O	-47.54	-29.71	65.19	15.00
5 VAL N	-45.68	-28.72	64.36	15.00
5 VAL CA	-45.14	-28.35	65.65	15.00
5 VAL CB	-44.25	-29.47	66.25	15.00
5 VAL CG1	-43.09	-29.81	65.33	15.00
5 VAL CG2	-43.75	-29.04	67.62	15.00
5 VAL C	-44.36	-27.06	65.44	15.00
5 VAL O	-43.60	-26.93	64.48	15.00
6 ASP N	-44.59	-26.08	66.30	15.00
6 ASP CA	-43.94	-24.79	66.20	15.00

TABLE III

6 ASP CB	-44.95	-23.76	65.68	15.00
6 ASP CG	-44.35	-22.38	65.47	15.00
6 ASP OD1	-43.14	-22.26	65.21	15.00
6 ASP OD2	-45.11	-21.39	65.56	15.00
6 ASP C	-43.47	-24.45	67.60	15.00
6 ASP O	-44.25	-24.02	68.45	15.00
7 TYR N	-42.18	-24.61	67.86	15.00
7 TYR CA	-41.62	-24.34	69.18	15.00
7 TYR CB	-40.24	-24.98	69.29	15.00
7 TYR CG	-40.34	-26.48	69.38	15.00
7 TYR CD1	-40.73	-27.10	70.57	15.00
7 TYR CE1	-40.88	-28.46	70.65	15.00
7 TYR CD2	-40.08	-27.28	68.27	15.00
7 TYR CE2	-40.23	-28.65	68.34	15.00
7 TYR CZ	-40.63	-29.23	69.53	15.00
7 TYR OH	-40.78	-30.58	69.62	15.00
7 TYR C	-41.58	-22.91	69.65	15.00
7 TYR O	-41.37	-22.64	70.84	15.00
8 ARG N	-41.80	-21.97	68.74	15.00
8 ARG CA	-41.78	-20.56	69.11	15.00
8 ARG CB	-41.99	-19.67	67.87	15.00
8 ARG CG	-40.88	-19.77	66.84	15.00
8 ARG CD	-41.23	-19.01	65.57	15.00
8 ARG NE	-42.50	-19.45	65.01	15.00
8 ARG CZ	-42.96	-19.10	63.81	15.00
8 ARG NH1	-42.24	-18.30	63.03	15.00
8 ARG NH2	-44.15	-19.53	63.40	15.00
8 ARG C	-42.85	-20.28	70.15	15.00
8 ARG O	-42.57	-19.72	71.21	15.00
9 LYS N	-44.06	-20.77	69.88	15.00
9 LYS CA	-45.18	-20.55	70.78	15.00
9 LYS CB	-46.50	-20.64	70.02	15.00
9 LYS CG	-46.63	-21.81	69.10	15.00
9 LYS CD	-47.93	-21.71	68.33	15.00
9 LYS CE	-48.22	-22.99	67.54	15.00
9 LYS NZ	-49.52	-22.90	66.80	15.00
9 LYS C	-45.22	-21.43	72.02	15.00
9 LYS O	-46.25	-21.56	72.67	15.00
10 LYS N	-44.08	-22.02	72.38	15.00
10 LYS CA	-43.97	-22.87	73.56	15.00
10 LYS CB	-43.66	-24.32	73.16	15.00
10 LYS CG	-44.79	-25.04	72.44	15.00
10 LYS CD	-44.37	-26.46	72.08	15.00

TABLE III

10	LYS	CE	-45.44	-27.16	71.27	15.00
10	LYS	NZ	-45.80	-26.44	70.01	15.00
10	LYS	C	-42.90	-22.38	74.54	15.00
10	LYS	O	-42.69	-22.99	75.59	15.00
11	GLY	N	-42.19	-21.30	74.19	15.00
11	GLY	CA	-41.15	-20.78	75.05	15.00
11	GLY	C	-39.83	-21.52	74.90	15.00
11	GLY	O	-38.95	-21.41	75.74	15.00
12	TYR	N	-39.69	-22.25	73.79	15.00
12	TYR	CA	-38.48	-23.03	73.51	15.00
12	TYR	CB	-38.82	-24.26	72.67	15.00
12	TYR	CG	-39.21	-25.54	73.39	15.00
12	TYR	CD1	-40.43	-25.65	74.06	15.00
12	TYR	CE1	-40.85	-26.87	74.58	15.00
12	TYR	CD2	-38.41	-26.68	73.27	15.00
12	TYR	CE2	-38.83	-27.90	73.79	15.00
12	TYR	CZ	-40.05	-27.98	74.44	15.00
12	TYR	OH	-40.47	-29.19	74.93	15.00
12	TYR	C	-37.45	-22.25	72.72	15.00
12	TYR	O	-36.33	-22.72	72.54	15.00
13	VAL	N	-37.85	-21.09	72.19	15.00
13	VAL	CA	-36.94	-20.29	71.37	15.00
13	VAL	CB	-37.40	-20.32	69.88	15.00
13	VAL	CG1	-38.59	-19.43	69.67	15.00
13	VAL	CG2	-36.26	-19.93	68.97	15.00
13	VAL	C	-36.77	-18.86	71.87	15.00
13	VAL	O	-37.69	-18.26	72.43	15.00
14	THR	N	-35.55	-18.35	71.69	15.00
14	THR	CA	-35.15	-17.00	72.11	15.00
14	THR	CB	-33.72	-17.00	72.67	15.00
14	THR	OG1	-32.83	-17.53	71.69	15.00
14	THR	CG2	-33.64	-17.86	73.91	15.00
14	THR	C	-35.21	-15.98	70.97	15.00
14	THR	O	-35.26	-16.36	69.81	15.00
15	PRO	N	-35.22	-14.68	71.31	15.00
15	PRO	CD	-35.25	-14.08	72.65	15.00
15	PRO	CA	-35.27	-13.64	70.28	15.00
15	PRO	CB	-35.03	-12.35	71.08	15.00
15	PRO	CG	-34.46	-12.83	72.43	15.00
15	PRO	C	-34.23	-13.82	69.17	15.00
15	PRO	O	-33.14	-14.35	69.41	15.00
16	VAL	N	-34.60	-13.42	67.96	15.00
16	VAL	CA	-33.72	-13.53	66.81	15.00

TABLE III

16 VAL CB	-34.45	-13.16	65.50	15.00
16 VAL CG1	-33.63	-13.60	64.31	15.00
16 VAL CG2	-35.81	-13.78	65.47	15.00
16 VAL C	-32.52	-12.61	66.97	15.00
16 VAL O	-32.67	-11.42	67.25	15.00
17 LYS N	-31.32	-13.17	66.80	15.00
17 LYS CA	-30.09	-12.42	66.91	15.00
17 LYS CB	-29.08	-13.18	67.77	15.00
17 LYS CG	-29.01	-12.72	69.22	15.00
17 LYS CD	-30.27	-13.09	70.02	15.00
17 LYS CE	-30.18	-14.48	70.64	15.00
17 LYS NZ	-29.12	-14.54	71.68	15.00
17 LYS C	-29.49	-12.15	65.54	15.00
17 LYS O	-29.82	-12.81	64.56	15.00
18 ASN N	-28.62	-11.15	65.49	15.00
18 ASN CA	-27.91	-10.77	64.27	15.00
18 ASN CB	-28.01	-9.26	64.05	15.00
18 ASN CG	-27.09	-8.78	62.94	15.00
18 ASN OD1	-26.98	-9.42	61.89	15.00
18 ASN ND2	-26.38	-7.69	63.19	15.00
18 ASN C	-26.45	-11.16	64.43	15.00
18 ASN O	-25.79	-10.73	65.37	15.00
19 GLN N	-25.94	-11.96	63.51	15.00
19 GLN CA	-24.56	-12.40	63.60	15.00
19 GLN CB	-24.34	-13.65	62.77	15.00
19 GLN CG	-24.88	-13.58	61.37	15.00
19 GLN CD	-24.42	-14.73	60.53	15.00
19 GLN OE1	-25.17	-15.28	59.73	15.00
19 GLN NE2	-23.15	-15.09	60.68	15.00
19 GLN C	-23.52	-11.35	63.24	15.00
19 GLN O	-22.35	-11.49	63.60	15.00
20 GLY N	-23.94	-10.31	62.53	15.00
20 GLY CA	-23.02	-9.26	62.14	15.00
20 GLY C	-22.10	-9.67	61.00	15.00
20 GLY O	-22.51	-10.40	60.11	15.00
21 GLN N	-20.85	-9.20	61.04	15.00
21 GLN CA	-19.86	-9.50	60.01	15.00
21 GLN CB	-18.92	-8.30	59.78	15.00
21 GLN CG	-19.60	-6.94	59.55	15.00
21 GLN CD	-20.68	-6.99	58.49	15.00
21 GLN OE1	-20.49	-7.53	57.41	15.00
21 GLN NE2	-21.85	-6.43	58.81	15.00
21 GLN C	-19.03	-10.74	60.38	15.00

TABLE III

21 GLN O	-18.02	-11.06	59.74	15.00
22 CYS N	-19.41	-11.42	61.44	15.00
22 CYS CA	-18.69	-12.60	61.88	15.00
22 CYS C	-19.37	-13.86	61.33	15.00
22 CYS O	-20.59	-13.94	61.27	15.00
22 CYS CB	-18.63	-12.61	63.41	15.00
22 CYS SG	-17.84	-14.05	64.16	15.00
23 GLY N	-18.58	-14.81	60.84	15.00
23 GLY CA	-19.15	-16.03	60.30	15.00
23 GLY C	-19.41	-17.03	61.41	15.00
23 GLY O	-18.90	-18.15	61.38	15.00
24 SER N	-20.22	-16.62	62.37	15.00
24 SER CA	-20.56	-17.43	63.53	15.00
24 SER CB	-20.36	-16.59	64.79	15.00
24 SER OG	-21.14	-15.41	64.68	15.00
24 SER C	-21.99	-17.95	63.49	15.00
24 SER O	-22.60	-18.20	64.53	15.00
25 CYS N	-22.55	-18.14	62.30	15.00
25 CYS CA	-23.91	-18.65	62.20	15.00
25 CYS CB	-24.41	-18.63	60.75	15.00
25 CYS SG	-23.48	-19.60	59.54	15.00
25 CYS C	-23.96	-20.05	62.82	15.00
25 CYS O	-24.97	-20.45	63.40	15.00
25 INH C1	-27.24	-9.28	57.72	15.00
25 INH C2	-26.55	-9.60	58.90	15.00
25 INH C3	-25.31	-10.22	58.84	15.00
25 INH C4	-24.73	-10.54	57.61	15.00
25 INH C5	-25.43	-10.21	56.44	15.00
25 INH C6	-26.67	-9.59	56.49	15.00
25 INH C7	-23.41	-11.26	57.54	15.00
25 INH O8	-23.43	-12.63	57.98	15.00
25 INH C9	-22.90	-13.56	57.08	15.00
25 INH O10	-21.75	-13.43	56.65	15.00
25 INH C11	-23.40	-15.62	55.77	15.00
25 INH C12	-22.32	-15.20	54.77	15.00
25 INH C13	-22.79	-14.65	53.42	15.00
25 INH C14	-21.66	-14.80	52.41	15.00
25 INH C15	-24.07	-15.33	52.91	15.00
25 INH C16	-23.13	-17.06	56.23	15.00
25 INH O17	-23.79	-17.98	55.74	15.00
25 INH N18	-22.17	-17.29	57.12	15.00
25 INH C19	-21.81	-18.63	57.60	15.00
25 INH N20	-23.72	-14.55	56.73	15.00

TABLE III

25	INH	C21	-21.96	-18.81	59.10	15.00
25	INH	O22	-21.89	-17.72	59.66	15.00
25	INH	C23	-19.42	-29.07	54.27	15.00
25	INH	C24	-20.11	-28.05	54.90	15.00
25	INH	C25	-19.45	-26.88	55.23	15.00
25	INH	C26	-18.09	-26.70	54.93	15.00
25	INH	C27	-17.41	-27.74	54.30	15.00
25	INH	C28	-18.06	-28.92	53.96	15.00
25	INH	C29	-17.39	-25.41	55.26	15.00
25	INH	O30	-18.05	-24.15	55.06	15.00
25	INH	C31	-19.20	-23.80	55.81	15.00
25	INH	O32	-20.33	-23.84	55.32	15.00
25	INH	C33	-20.15	-23.05	57.92	15.00
25	INH	C34	-20.47	-24.13	58.95	15.00
25	INH	C35	-21.49	-25.18	58.56	15.00
25	INH	C36	-22.36	-24.69	57.40	15.00
25	INH	C37	-20.73	-26.42	58.16	15.00
25	INH	C38	-19.89	-21.74	58.63	15.00
25	INH	O39	-18.75	-21.39	58.90	15.00
25	INH	N40	-20.97	-21.01	58.95	15.00
25	INH	C41	-20.91	-19.72	59.64	15.00
25	INH	N42	-19.01	-23.44	57.08	15.00
26	TRP	N	-22.84	-20.77	62.76	15.00
26	TRP	CA	-22.76	-22.11	63.33	15.00
26	TRP	CB	-21.47	-22.81	62.88	15.00
26	TRP	CG	-20.24	-22.16	63.40	15.00
26	TRP	CD2	-19.56	-22.46	64.62	15.00
26	TRP	CE2	-18.51	-21.53	64.75	15.00
26	TRP	CE3	-19.74	-23.42	65.63	15.00
26	TRP	CD1	-19.59	-21.11	62.84	15.00
26	TRP	NE1	-18.55	-20.72	63.65	15.00
26	TRP	CZ2	-17.64	-21.52	65.85	15.00
26	TRP	CZ3	-18.88	-23.42	66.72	15.00
26	TRP	CH2	-17.84	-22.47	66.82	15.00
26	TRP	C	-22.82	-22.02	64.87	15.00
26	TRP	O	-23.31	-22.93	65.53	15.00
27	ALA	N	-22.34	-20.92	65.44	15.00
27	ALA	CA	-22.36	-20.73	66.89	15.00
27	ALA	CB	-21.43	-19.61	67.30	15.00
27	ALA	C	-23.79	-20.43	67.32	15.00
27	ALA	O	-24.29	-21.00	68.29	15.00
28	PHE	N	-24.48	-19.57	66.58	15.00
28	PHE	CA	-25.85	-19.25	66.92	15.00

TABLE III

28 PHE CB	-26.38	-18.14	66.01	15.00
28 PHE CG	-25.87	-16.78	66.39	15.00
28 PHE CD1	-24.63	-16.33	65.94	15.00
28 PHE CD2	-26.61	-15.96	67.22	15.00
28 PHE CE1	-24.14	-15.10	66.33	15.00
28 PHE CE2	-26.11	-14.72	67.62	15.00
28 PHE CZ	-24.88	-14.29	67.17	15.00
28 PHE C	-26.73	-20.49	66.83	15.00
28 PHE O	-27.48	-20.80	67.75	15.00
29 SER N	-26.60	-21.24	65.74	15.00
29 SER CA	-27.36	-22.46	65.54	15.00
29 SER CB	-26.91	-23.14	64.25	15.00
29 SER OG	-27.55	-24.39	64.08	15.00
29 SER C	-27.17	-23.43	66.70	15.00
29 SER O	-28.14	-23.89	67.30	15.00
30 SER N	-25.91	-23.75	67.01	15.00
30 SER CA	-25.57	-24.67	68.09	15.00
30 SER CB	-24.06	-24.68	68.33	15.00
30 SER OG	-23.33	-25.06	67.19	15.00
30 SER C	-26.28	-24.24	69.38	15.00
30 SER O	-27.01	-25.02	70.01	15.00
31 VAL N	-26.09	-22.97	69.73	15.00
31 VAL CA	-26.67	-22.39	70.93	15.00
31 VAL CB	-26.13	-20.95	71.14	15.00
31 VAL CG1	-27.14	-20.07	71.79	15.00
31 VAL CG2	-24.87	-20.99	71.99	15.00
31 VAL C	-28.21	-22.46	70.89	15.00
31 VAL O	-28.86	-22.68	71.92	15.00
32 GLY N	-28.79	-22.36	69.70	15.00
32 GLY CA	-30.23	-22.42	69.58	15.00
32 GLY C	-30.77	-23.77	69.99	15.00
32 GLY O	-31.84	-23.88	70.58	15.00
33 ALA N	-30.04	-24.83	69.66	15.00
33 ALA CA	-30.46	-26.18	70.01	15.00
33 ALA CB	-29.67	-27.20	69.23	15.00
33 ALA C	-30.27	-26.36	71.50	15.00
33 ALA O	-31.10	-26.99	72.17	15.00
34 LEU N	-29.20	-25.80	72.04	15.00
34 LEU CA	-28.91	-25.88	73.47	15.00
34 LEU CB	-27.55	-25.25	73.77	15.00
34 LEU CG	-26.35	-26.14	73.47	15.00
34 LEU CD1	-25.07	-25.37	73.60	15.00
34 LEU CD2	-26.34	-27.30	74.42	15.00

TABLE III

34	LEU C	-30.00	-25.20	74.29	15.00
34	LEU O	-30.37	-25.66	75.38	15.00
35	GLU N	-30.56	-24.10	73.78	15.00
35	GLU CA	-31.61	-23.39	74.49	15.00
35	GLU CB	-31.82	-22.00	73.88	15.00
35	GLU CG	-30.62	-21.08	74.05	15.00
35	GLU CD	-30.60	-19.92	73.08	15.00
35	GLU OE1	-31.49	-19.83	72.21	15.00
35	GLU OE2	-29.66	-19.10	73.17	15.00
35	GLU C	-32.91	-24.18	74.47	15.00
35	GLU O	-33.62	-24.26	75.47	15.00
36	GLY N	-33.21	-24.80	73.33	15.00
36	GLY CA	-34.43	-25.58	73.22	15.00
36	GLY C	-34.49	-26.72	74.22	15.00
36	GLY O	-35.52	-26.94	74.86	15.00
37	GLN N	-33.38	-27.43	74.36	15.00
37	GLN CA	-33.27	-28.55	75.29	15.00
37	GLN CB	-31.99	-29.34	75.02	15.00
37	GLN CG	-32.04	-30.08	73.69	15.00
37	GLN CD	-33.27	-30.95	73.58	15.00
37	GLN OE1	-33.55	-31.77	74.45	15.00
37	GLN NE2	-34.04	-30.77	72.52	15.00
37	GLN C	-33.31	-28.07	76.74	15.00
37	GLN O	-33.94	-28.69	77.60	15.00
38	LEU N	-32.66	-26.94	77.00	15.00
38	LEU CA	-32.66	-26.34	78.34	15.00
38	LEU CB	-31.99	-24.97	78.30	15.00
38	LEU CG	-31.70	-24.28	79.63	15.00
38	LEU CD1	-30.58	-25.02	80.35	15.00
38	LEU CD2	-31.32	-22.84	79.40	15.00
38	LEU C	-34.11	-26.19	78.79	15.00
38	LEU O	-34.52	-26.71	79.82	15.00
39	LYS N	-34.91	-25.51	77.97	15.00
39	LYS CA	-36.31	-25.29	78.27	15.00
39	LYS CB	-36.98	-24.53	77.12	15.00
39	LYS CG	-38.48	-24.37	77.25	15.00
39	LYS CD	-38.89	-23.62	78.49	15.00
39	LYS CE	-40.38	-23.44	78.51	15.00
39	LYS NZ	-40.84	-22.84	79.78	15.00
39	LYS C	-37.01	-26.62	78.50	15.00
39	LYS O	-37.78	-26.76	79.44	15.00
40	LYS N	-36.70	-27.62	77.68	15.00
40	LYS CA	-37.32	-28.93	77.83	15.00

TABLE III

40	LYS	CB	-36.78	-29.89	76.76	15.00
40	LYS	CG	-37.56	-31.18	76.57	15.00
40	LYS	CD	-36.89	-32.09	75.54	15.00
40	LYS	CE	-37.73	-33.32	75.24	15.00
40	LYS	NZ	-39.05	-32.97	74.63	15.00
40	LYS	C	-37.07	-29.52	79.22	15.00
40	LYS	O	-38.00	-29.92	79.93	15.00
41	LYS	N	-35.80	-29.51	79.64	15.00
41	LYS	CA	-35.41	-30.07	80.92	15.00
41	LYS	CB	-33.92	-30.40	80.91	15.00
41	LYS	CG	-33.48	-31.19	79.67	15.00
41	LYS	CD	-34.36	-32.41	79.42	15.00
41	LYS	CE	-34.05	-33.08	78.08	15.00
41	LYS	NZ	-34.99	-34.21	77.78	15.00
41	LYS	C	-35.76	-29.21	82.13	15.00
41	LYS	O	-36.58	-29.61	82.96	15.00
42	THR	N	-35.17	-28.02	82.25	15.00
42	THR	CA	-35.41	-27.14	83.39	15.00
42	THR	CB	-34.27	-26.12	83.52	15.00
42	THR	OG1	-34.29	-25.25	82.38	15.00
42	THR	CG2	-32.94	-26.82	83.57	15.00
42	THR	C	-36.72	-26.37	83.39	15.00
42	THR	O	-37.10	-25.79	84.41	15.00
43	GLY	N	-37.40	-26.33	82.25	15.00
43	GLY	CA	-38.65	-25.60	82.15	15.00
43	GLY	C	-38.47	-24.08	82.03	15.00
43	GLY	O	-39.43	-23.33	81.98	15.00
44	LYS	N	-37.24	-23.57	82.01	15.00
44	LYS	CA	-37.05	-22.13	81.89	15.00
44	LYS	CB	-36.55	-21.53	83.20	15.00
44	LYS	CG	-37.49	-21.67	84.38	15.00
44	LYS	CD	-36.91	-20.99	85.61	15.00
44	LYS	CE	-35.68	-21.70	86.11	15.00
44	LYS	NZ	-36.03	-23.03	86.65	15.00
44	LYS	C	-36.05	-21.83	80.80	15.00
44	LYS	O	-35.00	-22.48	80.70	15.00
45	LEU	N	-36.39	-20.84	79.97	15.00
45	LEU	CA	-35.55	-20.41	78.86	15.00
45	LEU	CB	-36.43	-19.88	77.73	15.00
45	LEU	CG	-35.82	-19.71	76.33	15.00
45	LEU	CD1	-35.62	-21.08	75.69	15.00
45	LEU	CD2	-36.74	-18.87	75.48	15.00
45	LEU	C	-34.58	-19.34	79.32	15.00

TABLE III

45 LEU O	-34.92	-18.47	80.13	15.00
46 LEU N	-33.36	-19.39	78.80	15.00
46 LEU CA	-32.32	-18.44	79.15	15.00
46 LEU CB	-31.47	-19.02	80.28	15.00
46 LEU CG	-30.58	-18.14	81.17	15.00
46 LEU CD1	-29.23	-17.96	80.55	15.00
46 LEU CD2	-31.23	-16.81	81.44	15.00
46 LEU C	-31.51	-18.26	77.86	15.00
46 LEU O	-31.48	-19.15	77.01	15.00
47 ASN N	-30.92	-17.08	77.67	15.00
47 ASN CA	-30.14	-16.82	76.47	15.00
47 ASN CB	-30.22	-15.35	76.06	15.00
47 ASN CG	-31.33	-15.09	75.06	15.00
47 ASN OD1	-32.44	-14.74	75.43	15.00
47 ASN ND2	-31.04	-15.28	73.78	15.00
47 ASN C	-28.69	-17.26	76.64	15.00
47 ASN O	-27.98	-16.75	77.50	15.00
48 LEU N	-28.27	-18.21	75.82	15.00
48 LEU CA	-26.92	-18.73	75.89	15.00
48 LEU CB	-26.89	-20.21	75.51	15.00
48 LEU CG	-27.53	-21.15	76.55	15.00
48 LEU CD1	-27.34	-22.60	76.17	15.00
48 LEU CD2	-26.88	-20.92	77.88	15.00
48 LEU C	-25.93	-17.89	75.07	15.00
48 LEU O	-26.32	-17.11	74.20	15.00
49 SER N	-24.64	-18.08	75.35	15.00
49 SER CA	-23.56	-17.34	74.70	15.00
49 SER CB	-22.47	-17.07	75.75	15.00
49 SER OG	-21.31	-16.50	75.18	15.00
49 SER C	-22.92	-17.91	73.43	15.00
49 SER O	-22.16	-18.88	73.48	15.00
50 PRO N	-23.22	-17.30	72.26	15.00
50 PRO CD	-24.28	-16.31	72.02	15.00
50 PRO CA	-22.65	-17.75	70.98	15.00
50 PRO CB	-23.42	-16.92	69.95	15.00
50 PRO CG	-24.70	-16.64	70.62	15.00
50 PRO C	-21.16	-17.38	70.95	15.00
50 PRO O	-20.34	-18.08	70.35	15.00
51 GLN N	-20.81	-16.27	71.59	15.00
51 GLN CA	-19.43	-15.80	71.65	15.00
51 GLN CB	-19.35	-14.43	72.34	15.00
51 GLN CG	-17.95	-13.79	72.39	15.00
51 GLN CD	-17.46	-13.23	71.05	15.00

TABLE III

51 GLN OE1	-18.21	-12.62	70.30	15.00
51 GLN NE2	-16.19	-13.42	70.77	15.00
51 GLN C	-18.58	-16.83	72.38	15.00
51 GLN O	-17.46	-17.15	71.96	15.00
52 ASN N	-19.13	-17.42	73.44	15.00
52 ASN CA	-18.41	-18.42	74.24	15.00
52 ASN CB	-19.31	-18.96	75.35	15.00
52 ASN CG	-18.59	-19.90	76.31	15.00
52 ASN OD1	-19.23	-20.62	77.07	15.00
52 ASN ND2	-17.27	-19.89	76.28	15.00
52 ASN C	-17.91	-19.55	73.35	15.00
52 ASN O	-16.84	-20.12	73.59	15.00
53 LEU N	-18.67	-19.86	72.31	15.00
53 LEU CA	-18.33	-20.90	71.35	15.00
53 LEU CB	-19.58	-21.37	70.60	15.00
53 LEU CG	-20.63	-22.10	71.42	15.00
53 LEU CD1	-21.81	-22.44	70.55	15.00
53 LEU CD2	-20.01	-23.36	72.01	15.00
53 LEU C	-17.31	-20.42	70.34	15.00
53 LEU O	-16.37	-21.13	69.99	15.00
54 VAL N	-17.52	-19.19	69.87	15.00
54 VAL CA	-16.66	-18.57	68.87	15.00
54 VAL CB	-17.16	-17.14	68.56	15.00
54 VAL CG1	-16.22	-16.45	67.59	15.00
54 VAL CG2	-18.57	-17.20	68.00	15.00
54 VAL C	-15.20	-18.52	69.30	15.00
54 VAL O	-14.31	-18.88	68.53	15.00
55 ASP N	-14.96	-18.09	70.54	15.00
55 ASP CA	-13.61	-17.98	71.07	15.00
55 ASP CB	-13.58	-16.93	72.18	15.00
55 ASP CG	-14.14	-15.59	71.76	15.00
55 ASP OD1	-14.26	-15.33	70.55	15.00
55 ASP OD2	-14.45	-14.78	72.67	15.00
55 ASP C	-13.02	-19.26	71.65	15.00
55 ASP O	-11.80	-19.39	71.72	15.00
56 CYS N	-13.86	-20.19	72.09	15.00
56 CYS CA	-13.36	-21.41	72.73	15.00
56 CYS C	-13.29	-22.71	71.94	15.00
56 CYS O	-12.43	-23.55	72.20	15.00
56 CYS CB	-14.10	-21.61	74.04	15.00
56 CYS SG	-14.21	-20.10	75.06	15.00
57 VAL N	-14.17	-22.93	70.96	15.00
57 VAL CA	-14.13	-24.17	70.18	15.00

TABLE III

57 VAL CB	-15.44	-24.43	69.39	15.00
57 VAL CG1	-15.38	-25.80	68.73	15.00
57 VAL CG2	-16.63	-24.33	70.30	15.00
57 VAL C	-12.97	-24.10	69.19	15.00
57 VAL O	-13.17	-23.81	68.02	15.00
58 SER N	-11.76	-24.40	69.66	15.00
58 SER CA	-10.57	-24.35	68.82	15.00
58 SER CB	-9.34	-24.73	69.63	15.00
58 SER OG	-9.44	-26.08	70.07	15.00
58 SER C	-10.65	-25.25	67.61	15.00
58 SER O	-9.90	-25.09	66.65	15.00
59 GLU N	-11.53	-26.25	67.65	15.00
59 GLU CA	-11.69	-27.16	66.53	15.00
59 GLU CB	-12.57	-28.35	66.92	15.00
59 GLU CG	-12.00	-29.23	68.00	15.00
59 GLU CD	-11.98	-28.56	69.36	15.00
59 GLU OE1	-13.00	-27.95	69.73	15.00
59 GLU OE2	-10.95	-28.66	70.06	15.00
59 GLU C	-12.30	-26.41	65.35	15.00
59 GLU O	-12.28	-26.89	64.22	15.00
60 ASN N	-12.89	-25.26	65.63	15.00
60 ASN CA	-13.53	-24.45	64.61	15.00
60 ASN CB	-14.95	-24.06	65.03	15.00
60 ASN CG	-15.92	-25.21	64.90	15.00
60 ASN OD1	-17.09	-25.08	65.23	15.00
60 ASN ND2	-15.45	-26.34	64.38	15.00
60 ASN C	-12.71	-23.22	64.26	15.00
60 ASN O	-11.73	-22.92	64.93	15.00
61 ASP N	-13.13	-22.50	63.23	15.00
61 ASP CA	-12.41	-21.34	62.75	15.00
61 ASP CB	-12.53	-21.28	61.22	15.00
61 ASP CG	-11.20	-21.01	60.53	15.00
61 ASP OD1	-10.34	-20.32	61.12	15.00
61 ASP OD2	-11.03	-21.49	59.40	15.00
61 ASP C	-12.80	-19.99	63.35	15.00
61 ASP O	-12.23	-18.95	62.99	15.00
62 GLY N	-13.75	-19.97	64.28	15.00
62 GLY CA	-14.17	-18.71	64.87	15.00
62 GLY C	-15.12	-18.03	63.91	15.00
62 GLY O	-16.13	-18.61	63.51	15.00
63 CYS N	-14.80	-16.81	63.48	15.00
63 CYS CA	-15.65	-16.09	62.52	15.00
63 CYS C	-15.45	-16.63	61.12	15.00

TABLE III

63 CYS O	-16.10	-16.16	60.18	15.00
63 CYS CB	-15.34	-14.59	62.52	15.00
63 CYS SG	-15.84	-13.72	64.03	15.00
64 GLY N	-14.52	-17.56	60.95	15.00
64 GLY CA	-14.26	-18.14	59.65	15.00
64 GLY C	-15.17	-19.33	59.40	15.00
64 GLY O	-15.50	-19.67	58.26	15.00
65 GLY N	-15.60	-19.99	60.48	15.00
65 GLY CA	-16.47	-21.14	60.33	15.00
65 GLY C	-16.39	-22.20	61.41	15.00
65 GLY O	-15.56	-22.15	62.31	15.00
66 GLY N	-17.28	-23.18	61.30	15.00
66 GLY CA	-17.31	-24.25	62.27	15.00
66 GLY C	-18.50	-25.16	62.14	15.00
66 GLY O	-19.48	-24.83	61.48	15.00
67 TYR N	-18.43	-26.32	62.78	15.00
67 TYR CA	-19.51	-27.30	62.74	15.00
67 TYR CB	-18.97	-28.70	62.45	15.00
67 TYR CG	-18.28	-28.86	61.12	15.00
67 TYR CD1	-19.02	-29.00	59.94	15.00
67 TYR CE1	-18.40	-29.23	58.72	15.00
67 TYR CD2	-16.90	-28.94	61.04	15.00
67 TYR CE2	-16.26	-29.16	59.82	15.00
67 TYR CZ	-17.02	-29.31	58.67	15.00
67 TYR OH	-16.39	-29.51	57.46	15.00
67 TYR C	-20.17	-27.29	64.10	15.00
67 TYR O	-19.48	-27.14	65.12	15.00
68 MET N	-21.48	-27.47	64.12	15.00
68 MET CA	-22.26	-27.48	65.36	15.00
68 MET CB	-23.76	-27.60	65.07	15.00
68 MET CG	-24.38	-26.42	64.29	15.00
68 MET SD	-23.94	-26.32	62.55	15.00
68 MET CE	-25.16	-27.35	61.83	15.00
68 MET C	-21.81	-28.62	66.27	15.00
68 MET O	-21.63	-28.43	67.47	15.00
69 THR N	-21.58	-29.79	65.68	15.00
69 THR CA	-21.15	-30.96	66.43	15.00
69 THR CB	-20.90	-32.18	65.50	15.00
69 THR OG1	-20.04	-31.81	64.42	15.00
69 THR CG2	-22.21	-32.71	64.94	15.00
69 THR C	-19.90	-30.65	67.25	15.00
69 THR O	-19.80	-31.06	68.41	15.00
70 ASN N	-18.98	-29.86	66.69	15.00

TABLE III

70 ASN CA	-17.74	-29.49	67.37	15.00
70 ASN CB	-16.79	-28.76	66.42	15.00
70 ASN CG	-16.05	-29.71	65.50	15.00
70 ASN OD1	-14.84	-29.64	65.39	15.00
70 ASN ND2	-16.78	-30.58	64.83	15.00
70 ASN C	-18.01	-28.62	68.59	15.00
70 ASN O	-17.32	-28.74	69.60	15.00
71 ALA N	-19.03	-27.77	68.48	15.00
71 ALA CA	-19.43	-26.88	69.56	15.00
71 ALA CB	-20.37	-25.81	69.04	15.00
71 ALA C	-20.12	-27.68	70.67	15.00
71 ALA O	-20.03	-27.32	71.84	15.00
72 PHE N	-20.85	-28.72	70.28	15.00
72 PHE CA	-21.54	-29.59	71.22	15.00
72 PHE CB	-22.36	-30.65	70.47	15.00
72 PHE CG	-23.54	-30.11	69.74	15.00
72 PHE CD1	-24.28	-29.06	70.24	15.00
72 PHE CD2	-23.91	-30.66	68.53	15.00
72 PHE CE1	-25.36	-28.56	69.55	15.00
72 PHE CE2	-25.00	-30.17	67.83	15.00
72 PHE CZ	-25.72	-29.12	68.34	15.00
72 PHE C	-20.46	-30.29	72.05	15.00
72 PHE O	-20.43	-30.18	73.28	15.00
73 GLN N	-19.58	-30.98	71.34	15.00
73 GLN CA	-18.47	-31.71	71.92	15.00
73 GLN CB	-17.53	-32.13	70.78	15.00
73 GLN CG	-16.60	-33.30	71.06	15.00
73 GLN CD	-17.31	-34.63	71.03	15.00
73 GLN OE1	-17.80	-35.13	72.06	15.00
73 GLN NE2	-17.35	-35.25	69.85	15.00
73 GLN C	-17.74	-30.81	72.93	15.00
73 GLN O	-17.27	-31.26	73.97	15.00
74 TYR N	-17.66	-29.51	72.63	15.00
74 TYR CA	-17.00	-28.57	73.51	15.00
74 TYR CB	-16.75	-27.21	72.81	15.00
74 TYR CG	-16.41	-26.08	73.77	15.00
74 TYR CD1	-15.19	-26.05	74.43	15.00
74 TYR CE1	-14.91	-25.06	75.37	15.00
74 TYR CD2	-17.34	-25.09	74.06	15.00
74 TYR CE2	-17.07	-24.10	75.00	15.00
74 TYR CZ	-15.86	-24.09	75.66	15.00
74 TYR OH	-15.60	-23.15	76.63	15.00
74 TYR C	-17.75	-28.36	74.82	15.00

TABLE III

74 TYR O	-17.14	-28.37	75.89	15.00
75 VAL N	-19.07	-28.16	74.78	15.00
75 VAL CA	-19.85	-27.94	76.02	15.00
75 VAL CB	-21.30	-27.45	75.73	15.00
75 VAL CG1	-22.06	-27.23	77.04	15.00
75 VAL CG2	-21.27	-26.15	74.92	15.00
75 VAL C	-19.87	-29.20	76.91	15.00
75 VAL O	-20.07	-29.13	78.12	15.00
76 GLN N	-19.65	-30.35	76.29	15.00
76 GLN CA	-19.62	-31.60	77.01	15.00
76 GLN CB	-19.93	-32.73	76.04	15.00
76 GLN CG	-20.02	-34.11	76.67	15.00
76 GLN CD	-19.74	-35.20	75.68	15.00
76 GLN OE1	-20.14	-35.11	74.52	15.00
76 GLN NE2	-19.01	-36.22	76.11	15.00
76 GLN C	-18.25	-31.81	77.66	15.00
76 GLN O	-18.14	-32.17	78.85	15.00
77 LYS N	-17.18	-31.59	76.89	15.00
77 LYS CA	-15.82	-31.78	77.39	15.00
77 LYS CB	-14.83	-31.98	76.24	15.00
77 LYS CG	-14.56	-30.75	75.41	15.00
77 LYS CD	-13.69	-31.09	74.19	15.00
77 LYS CE	-14.41	-32.05	73.24	15.00
77 LYS NZ	-13.62	-32.45	72.02	15.00
77 LYS C	-15.34	-30.65	78.29	15.00
77 LYS O	-14.37	-30.81	79.01	15.00
78 ASN N	-15.97	-29.49	78.22	15.00
78 ASN CA	-15.60	-28.37	79.07	15.00
78 ASN CB	-15.58	-27.07	78.27	15.00
78 ASN CG	-15.38	-25.85	79.16	15.00
78 ASN OD1	-14.28	-25.58	79.64	15.00
78 ASN ND2	-16.45	-25.11	79.37	15.00
78 ASN C	-16.62	-28.28	80.20	15.00
78 ASN O	-16.36	-27.67	81.23	15.00
79 ARG N	-17.77	-28.91	79.97	15.00
79 ARG CA	-18.89	-28.98	80.92	15.00
79 ARG CB	-18.58	-29.92	82.11	15.00
79 ARG CG	-17.47	-29.49	83.06	15.00
79 ARG CD	-16.62	-30.66	83.51	15.00
79 ARG NE	-17.44	-31.76	84.00	15.00
79 ARG CZ	-17.90	-32.75	83.23	15.00
79 ARG NH1	-17.60	-32.77	81.93	15.00
79 ARG NH2	-18.73	-33.66	83.74	15.00

TABLE III

79 ARG C	-19.45	-27.65	81.39	15.00
79 ARG O	-19.42	-27.31	82.57	15.00
80 GLY N	-20.00	-26.92	80.44	15.00
80 GLY CA	-20.58	-25.63	80.75	15.00
80 GLY C	-20.41	-24.62	79.63	15.00
80 GLY O	-19.39	-24.61	78.93	15.00
81 ILE N	-21.44	-23.82	79.44	15.00
81 ILE CA	-21.45	-22.77	78.45	15.00
81 ILE CB	-22.27	-23.14	77.21	15.00
81 ILE CG2	-23.71	-23.46	77.59	15.00
81 ILE CG1	-22.18	-22.01	76.17	15.00
81 ILE CD1	-22.74	-22.34	74.79	15.00
81 ILE C	-22.09	-21.59	79.18	15.00
81 ILE O	-23.08	-21.77	79.89	15.00
82 ASP N	-21.48	-20.42	79.06	15.00
82 ASP CA	-21.99	-19.22	79.72	15.00
82 ASP CB	-20.95	-18.10	79.68	15.00
82 ASP CG	-19.75	-18.37	80.56	15.00
82 ASP OD1	-18.66	-17.89	80.20	15.00
82 ASP OD2	-19.89	-19.03	81.62	15.00
82 ASP C	-23.27	-18.70	79.09	15.00
82 ASP O	-23.67	-19.11	78.01	15.00
83 SER N	-23.91	-17.78	79.79	15.00
83 SER CA	-25.12	-17.15	79.30	15.00
83 SER CB	-26.03	-16.79	80.46	15.00
83 SER OG	-25.32	-16.05	81.44	15.00
83 SER C	-24.66	-15.90	78.58	15.00
83 SER O	-23.49	-15.51	78.67	15.00
84 GLU N	-25.57	-15.24	77.87	15.00
84 GLU CA	-25.22	-14.02	77.16	15.00
84 GLU CB	-26.40	-13.50	76.35	15.00
84 GLU CG	-26.09	-12.30	75.46	15.00
84 GLU CD	-25.06	-12.58	74.36	15.00
84 GLU OE1	-25.03	-13.69	73.78	15.00
84 GLU OE2	-24.28	-11.66	74.06	15.00
84 GLU C	-24.70	-12.95	78.14	15.00
84 GLU O	-23.64	-12.37	77.92	15.00
85 ASP N	-25.41	-12.69	79.23	15.00
85 ASP CA	-24.95	-11.70	80.20	15.00
85 ASP CB	-25.99	-11.46	81.31	15.00
85 ASP CG	-25.59	-10.32	82.30	15.00
85 ASP OD1	-26.24	-10.19	83.38	15.00
85 ASP OD2	-24.66	-9.54	82.02	15.00

TABLE III

85 ASP C	-23.63	-12.15	80.82	15.00
85 ASP O	-22.86	-11.34	81.34	15.00
86 ALA N	-23.31	-13.44	80.74	15.00
86 ALA CA	-22.07	-13.91	81.32	15.00
86 ALA CB	-22.24	-15.30	81.86	15.00
86 ALA C	-20.90	-13.85	80.35	15.00
86 ALA O	-19.74	-13.84	80.76	15.00
87 TYR N	-21.19	-13.82	79.05	15.00
87 TYR CA	-20.14	-13.77	78.03	15.00
87 TYR CB	-19.67	-15.20	77.77	15.00
87 TYR CG	-18.31	-15.36	77.13	15.00
87 TYR CD1	-17.86	-14.49	76.13	15.00
87 TYR CE1	-16.64	-14.70	75.51	15.00
87 TYR CD2	-17.49	-16.43	77.48	15.00
87 TYR CE2	-16.27	-16.64	76.86	15.00
87 TYR CZ	-15.85	-15.78	75.88	15.00
87 TYR OH	-14.65	-16.03	75.26	15.00
87 TYR C	-20.73	-13.17	76.75	15.00
87 TYR O	-20.92	-13.88	75.76	15.00
88 PRO N	-20.99	-11.84	76.74	15.00
88 PRO CD	-20.79	-10.92	77.87	15.00
88 PRO CA	-21.57	-11.12	75.60	15.00
88 PRO CB	-21.52	-9.66	76.07	15.00
88 PRO CG	-21.75	-9.80	77.54	15.00
88 PRO C	-20.91	-11.29	74.24	15.00
88 PRO O	-19.71	-11.56	74.13	15.00
89 TYR N	-21.72	-11.10	73.21	15.00
89 TYR CA	-21.30	-11.23	71.83	15.00
89 TYR CB	-22.51	-11.59	70.96	15.00
89 TYR CG	-22.16	-12.03	69.56	15.00
89 TYR CD1	-21.27	-13.09	69.35	15.00
89 TYR CE1	-20.90	-13.46	68.07	15.00
89 TYR CD2	-22.67	-11.37	68.45	15.00
89 TYR CE2	-22.31	-11.74	67.17	15.00
89 TYR CZ	-21.42	-12.78	66.98	15.00
89 TYR OH	-21.02	-13.12	65.72	15.00
89 TYR C	-20.67	-9.90	71.38	15.00
89 TYR O	-21.33	-8.86	71.36	15.00
90 VAL N	-19.38	-9.93	71.05	15.00
90 VAL CA	-18.66	-8.73	70.61	15.00
90 VAL CB	-17.25	-8.65	71.22	15.00
90 VAL CG1	-17.32	-8.67	72.73	15.00
90 VAL CG2	-16.37	-9.78	70.68	15.00

TABLE III

90 VAL C	-18.54	-8.62	69.11	15.00
90 VAL O	-17.85	-7.75	68.61	15.00
91 GLY N	-19.14	-9.55	68.39	15.00
91 GLY CA	-19.10	-9.49	66.94	15.00
91 GLY C	-17.76	-9.77	66.31	15.00
91 GLY O	-17.52	-9.39	65.15	15.00
92 GLN N	-16.88	-10.44	67.03	15.00
92 GLN CA	-15.56	-10.77	66.50	15.00
92 GLN CB	-14.74	-9.51	66.31	15.00
92 GLN CG	-14.49	-8.76	67.60	15.00
92 GLN CD	-13.93	-7.40	67.35	15.00
92 GLN OE1	-12.83	-7.06	67.80	15.00
92 GLN NE2	-14.67	-6.59	66.60	15.00
92 GLN C	-14.81	-11.73	67.41	15.00
92 GLN O	-15.19	-11.95	68.57	15.00
93 GLU N	-13.72	-12.26	66.89	15.00
93 GLU CA	-12.90	-13.22	67.59	15.00
93 GLU CB	-12.01	-13.95	66.59	15.00
93 GLU CG	-12.77	-14.60	65.42	15.00
93 GLU CD	-11.84	-15.07	64.31	15.00
93 GLU OE1	-10.67	-15.37	64.62	15.00
93 GLU OE2	-12.27	-15.13	63.13	15.00
93 GLU C	-12.05	-12.56	68.66	15.00
93 GLU O	-11.53	-11.46	68.49	15.00
94 GLU N	-11.92	-13.25	69.78	15.00
94 GLU CA	-11.13	-12.78	70.91	15.00
94 GLU CB	-11.93	-11.79	71.76	15.00
94 GLU CG	-13.39	-12.15	71.95	15.00
94 GLU CD	-14.00	-11.50	73.18	15.00
94 GLU OE1	-14.15	-10.26	73.18	15.00
94 GLU OE2	-14.31	-12.24	74.14	15.00
94 GLU C	-10.73	-13.98	71.74	15.00
94 GLU O	-11.15	-15.10	71.47	15.00
95 SER N	-9.88	-13.75	72.73	15.00
95 SER CA	-9.40	-14.80	73.61	15.00
95 SER CB	-8.39	-14.21	74.60	15.00
95 SER OG	-7.22	-13.77	73.94	15.00
95 SER C	-10.57	-15.44	74.35	15.00
95 SER O	-11.48	-14.73	74.82	15.00
96 CYS N	-10.55	-16.77	74.42	15.00
96 CYS CA	-11.59	-17.52	75.13	15.00
96 CYS C	-11.61	-17.01	76.56	15.00
96 CYS O	-10.57	-16.90	77.21	15.00

TABLE III

96 CYS CB	-11.31	-19.03	75.08	15.00
96 CYS SG	-12.44	-20.07	76.07	15.00
97 MET N	-12.80	-16.65	77.03	15.00
97 MET CA	-12.96	-16.09	78.36	15.00
97 MET CB	-13.24	-14.58	78.26	15.00
97 MET CG	-12.05	-13.75	77.73	15.00
97 MET SD	-12.56	-12.29	76.76	15.00
97 MET CE	-13.48	-11.34	78.03	15.00
97 MET C	-14.07	-16.78	79.14	15.00
97 MET O	-14.87	-16.11	79.82	15.00
98 TYR N	-14.13	-18.10	79.07	15.00
98 TYR CA	-15.15	-18.84	79.78	15.00
98 TYR CB	-15.00	-20.35	79.61	15.00
98 TYR CG	-16.06	-21.14	80.35	15.00
98 TYR CD1	-17.39	-21.10	79.94	15.00
98 TYR CE1	-18.38	-21.80	80.65	15.00
98 TYR CD2	-15.74	-21.90	81.48	15.00
98 TYR CE2	-16.72	-22.60	82.18	15.00
98 TYR CZ	-18.03	-22.54	81.76	15.00
98 TYR OH	-19.00	-23.23	82.44	15.00
98 TYR C	-15.08	-18.52	81.26	15.00
98 TYR O	-14.04	-18.68	81.89	15.00
99 ASN N	-16.19	-18.01	81.79	15.00
99 ASN CA	-16.31	-17.67	83.19	15.00
99 ASN CB	-16.96	-16.29	83.38	15.00
99 ASN CG	-17.25	-15.98	84.84	15.00
99 ASN OD1	-16.67	-16.58	85.75	15.00
99 ASN ND2	-18.19	-15.06	85.07	15.00
99 ASN C	-17.20	-18.74	83.81	15.00
99 ASN O	-18.44	-18.61	83.82	15.00
100 PRO N	-16.59	-19.79	84.39	15.00
100 PRO CD	-15.15	-19.84	84.68	15.00
100 PRO CA	-17.29	-20.92	85.02	15.00
100 PRO CB	-16.19	-21.58	85.86	15.00
100 PRO CG	-15.15	-20.47	86.03	15.00
100 PRO C	-18.50	-20.55	85.87	15.00
100 PRO O	-19.48	-21.29	85.92	15.00
101 THR N	-18.46	-19.40	86.53	15.00
101 THR CA	-19.58	-19.00	87.37	15.00
101 THR CB	-19.22	-17.77	88.22	15.00
101 THR OG1	-18.93	-16.65	87.36	15.00
101 THR CG2	-17.99	-18.06	89.08	15.00
101 THR C	-20.81	-18.70	86.52	15.00

TABLE III

101 THR O	-21.94	-19.07	86.88	15.00
102 GLY N	-20.59	-18.06	85.37	15.00
102 GLY CA	-21.68	-17.73	84.47	15.00
102 GLY C	-22.27	-18.92	83.72	15.00
102 GLY O	-23.16	-18.73	82.87	15.00
103 LYS N	-21.80	-20.14	84.00	15.00
103 LYS CA	-22.32	-21.34	83.33	15.00
103 LYS CB	-21.70	-22.60	83.93	15.00
103 LYS CG	-22.23	-23.88	83.33	15.00
103 LYS CD	-21.78	-25.11	84.11	15.00
103 LYS CE	-22.56	-25.26	85.40	15.00
103 LYS NZ	-24.02	-25.47	85.12	15.00
103 LYS C	-23.83	-21.42	83.45	15.00
103 LYS O	-24.39	-21.26	84.53	15.00
104 ALA N	-24.50	-21.68	82.34	15.00
104 ALA CA	-25.96	-21.77	82.34	15.00
104 ALA CB	-26.56	-20.57	81.61	15.00
104 ALA C	-26.48	-23.07	81.73	15.00
104 ALA O	-27.69	-23.30	81.71	15.00
105 ALA N	-25.59	-23.92	81.24	15.00
105 ALA CA	-26.02	-25.18	80.65	15.00
105 ALA CB	-26.71	-24.94	79.31	15.00
105 ALA C	-24.89	-26.20	80.49	15.00
105 ALA O	-23.72	-25.84	80.50	15.00
106 LYS N	-25.28	-27.46	80.37	15.00
106 LYS CA	-24.36	-28.59	80.21	15.00
106 LYS CB	-24.28	-29.40	81.51	15.00
106 LYS CG	-23.38	-28.89	82.62	15.00
106 LYS CD	-23.65	-29.73	83.87	15.00
106 LYS CE	-22.48	-29.72	84.85	15.00
106 LYS NZ	-21.33	-30.54	84.36	15.00
106 LYS C	-24.99	-29.49	79.16	15.00
106 LYS O	-26.18	-29.32	78.83	15.00
107 CYS N	-24.23	-30.42	78.61	15.00
107 CYS CA	-24.77	-31.37	77.64	15.00
107 CYS CB	-24.82	-30.77	76.22	15.00
107 CYS SG	-23.38	-31.03	75.18	15.00
107 CYS C	-23.93	-32.64	77.72	15.00
107 CYS O	-22.76	-32.59	78.10	15.00
108 ARG N	-24.54	-33.78	77.45	15.00
108 ARG CA	-23.86	-35.07	77.52	15.00
108 ARG CB	-24.60	-35.99	78.50	15.00
108 ARG CG	-26.12	-35.73	78.59	15.00

TABLE IV

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for the cathepsin K complex with inhibitor 2,2'-N,N'-bis-benzyloxycarbonyl-L-leucinylcarbohydrazide.

Residue Atom	X	Y	Z	B
1 ALA CB	-44.52	-37.54	64.26	15.00
1 ALA C	-46.72	-36.34	64.48	15.00
1 ALA O	-47.32	-36.96	63.59	15.00
1 ALA N	-46.03	-38.05	66.17	15.00
1 ALA CA	-45.55	-36.98	65.24	15.00
2 PRO N	-47.09	-35.10	64.86	15.00
2 PRO CD	-46.48	-34.27	65.92	15.00
2 PRO CA	-48.19	-34.39	64.20	15.00
2 PRO CB	-48.32	-33.13	65.04	15.00
2 PRO CG	-46.89	-32.89	65.50	15.00
2 PRO C	-47.85	-34.05	62.76	15.00
2 PRO O	-46.73	-34.29	62.29	15.00
3 ASP N	-48.84	-33.52	62.05	15.00
3 ASP CA	-48.64	-33.12	60.66	15.00
3 ASP CB	-49.97	-33.13	59.91	15.00
3 ASP CG	-50.31	-34.49	59.37	15.00
3 ASP OD1	-50.61	-34.58	58.16	15.00
3 ASP OD2	-50.25	-35.48	60.14	15.00
3 ASP C	-48.06	-31.73	60.63	15.00
3 ASP O	-47.45	-31.32	59.63	15.00
4 SER N	-48.18	-31.03	61.75	15.00
4 SER CA	-47.72	-29.67	61.87	15.00
4 SER CB	-48.86	-28.74	61.51	15.00
4 SER OG	-48.48	-27.37	61.57	15.00
4 SER C	-47.29	-29.41	63.29	15.00
4 SER O	-47.89	-29.91	64.23	15.00
5 VAL N	-46.20	-28.66	63.43	15.00
5 VAL CA	-45.71	-28.29	64.73	15.00
5 VAL CB	-44.98	-29.44	65.47	15.00
5 VAL CG1	-43.59	-29.68	64.89	15.00
5 VAL CG2	-44.88	-29.11	66.96	15.00
5 VAL C	-44.81	-27.08	64.62	15.00
5 VAL O	-44.04	-26.93	63.66	15.00
6 ASP N	-44.96	-26.20	65.59	15.00
6 ASP CA	-44.19	-24.98	65.66	15.00

TABLE IV

6 ASP CB	-45.08	-23.81	65.22	15.00
6 ASP CG	-44.31	-22.52	65.06	15.00
6 ASP OD1	-43.13	-22.45	65.49	15.00
6 ASP OD2	-44.88	-21.58	64.49	15.00
6 ASP C	-43.72	-24.81	67.10	15.00
6 ASP O	-44.50	-24.48	68.00	15.00
7 TYR N	-42.42	-25.02	67.31	15.00
7 TYR CA	-41.83	-24.90	68.64	15.00
7 TYR CB	-40.43	-25.53	68.66	15.00
7 TYR CG	-40.49	-27.05	68.76	15.00
7 TYR CD1	-40.75	-27.66	69.98	15.00
7 TYR CE1	-40.88	-29.04	70.08	15.00
7 TYR CD2	-40.34	-27.85	67.63	15.00
7 TYR CE2	-40.47	-29.24	67.72	15.00
7 TYR CZ	-40.74	-29.83	68.95	15.00
7 TYR OH	-40.89	-31.20	69.06	15.00
7 TYR C	-41.80	-23.47	69.20	15.00
7 TYR O	-41.66	-23.28	70.42	15.00
8 ARG N	-41.93	-22.48	68.33	15.00
8 ARG CA	-41.95	-21.08	68.77	15.00
8 ARG CB	-42.06	-20.12	67.58	15.00
8 ARG CG	-40.92	-20.21	66.57	15.00
8 ARG CD	-41.19	-19.30	65.38	15.00
8 ARG NE	-42.23	-19.84	64.51	15.00
8 ARG CZ	-42.66	-19.26	63.38	15.00
8 ARG NH1	-42.13	-18.11	62.97	15.00
8 ARG NH2	-43.61	-19.84	62.66	15.00
8 ARG C	-43.20	-20.93	69.64	15.00
8 ARG O	-43.18	-20.25	70.68	15.00
9 LYS N	-44.28	-21.58	69.21	15.00
9 LYS CA	-45.54	-21.53	69.92	15.00
9 LYS CB	-46.66	-22.14	69.08	15.00
9 LYS CG	-47.11	-21.26	67.92	15.00
9 LYS CD	-47.98	-22.07	66.95	15.00
9 LYS CE	-48.74	-21.20	65.98	15.00
9 LYS NZ	-49.84	-20.49	66.67	15.00
9 LYS C	-45.45	-22.22	71.27	15.00
9 LYS O	-46.19	-21.88	72.19	15.00
10 LYS N	-44.53	-23.16	71.39	15.00
10 LYS CA	-44.30	-23.91	72.63	15.00
10 LYS CB	-43.82	-25.33	72.30	15.00
10 LYS CG	-44.90	-26.25	71.75	15.00
10 LYS CD	-44.35	-27.64	71.47	15.00

TABLE IV

10	LYS	CE	-45.48	-28.63	71.20	15.00
10	LYS	NZ	-44.99	-30.01	70.87	15.00
10	LYS	C	-43.28	-23.22	73.53	15.00
10	LYS	O	-42.94	-23.73	74.60	15.00
11	GLY	N	-42.75	-22.09	73.09	15.00
11	GLY	CA	-41.77	-21.37	73.88	15.00
11	GLY	C	-40.41	-22.04	73.97	15.00
11	GLY	O	-39.71	-21.91	74.97	15.00
12	TYR	N	-40.02	-22.75	72.92	15.00
12	TYR	CA	-38.73	-23.41	72.89	15.00
12	TYR	CB	-38.86	-24.81	72.29	15.00
12	TYR	CG	-39.47	-25.86	73.18	15.00
12	TYR	CD1	-40.56	-25.59	73.99	15.00
12	TYR	CE1	-41.12	-26.56	74.81	15.00
12	TYR	CD2	-38.94	-27.15	73.21	15.00
12	TYR	CE2	-39.49	-28.14	74.02	15.00
12	TYR	CZ	-40.58	-27.84	74.82	15.00
12	TYR	OH	-41.10	-28.81	75.64	15.00
12	TYR	C	-37.73	-22.62	72.04	15.00
12	TYR	O	-36.65	-23.14	71.72	15.00
13	VAL	N	-38.08	-21.39	71.66	15.00
13	VAL	CA	-37.21	-20.59	70.80	15.00
13	VAL	CB	-37.82	-20.46	69.40	15.00
13	VAL	CG1	-36.75	-20.07	68.38	15.00
13	VAL	CG2	-38.52	-21.73	69.02	15.00
13	VAL	C	-36.93	-19.17	71.30	15.00
13	VAL	O	-37.86	-18.42	71.61	15.00
14	THR	N	-35.66	-18.79	71.34	15.00
14	THR	CA	-35.29	-17.45	71.78	15.00
14	THR	CB	-33.84	-17.40	72.32	15.00
14	THR	OG1	-32.91	-17.76	71.28	15.00
14	THR	CG2	-33.67	-18.33	73.52	15.00
14	THR	C	-35.46	-16.52	70.59	15.00
14	THR	O	-35.55	-16.96	69.46	15.00
15	PRO	N	-35.49	-15.20	70.84	15.00
15	PRO	CD	-35.39	-14.48	72.12	15.00
15	PRO	CA	-35.65	-14.27	69.72	15.00
15	PRO	CB	-35.71	-12.90	70.42	15.00
15	PRO	CG	-34.93	-13.12	71.67	15.00
15	PRO	C	-34.54	-14.35	68.69	15.00
15	PRO	O	-33.45	-14.89	68.95	15.00
16	VAL	N	-34.85	-13.85	67.50	15.00
16	VAL	CA	-33.94	-13.84	66.37	15.00

TABLE IV

16 VAL CB	-34.68	-13.41	65.08	15.00
16 VAL CG1	-33.72	-13.35	63.90	15.00
16 VAL CG2	-35.82	-14.39	64.78	15.00
16 VAL C	-32.71	-12.94	66.61	15.00
16 VAL O	-32.84	-11.79	67.04	15.00
17 LYS N	-31.54	-13.50	66.33	15.00
17 LYS CA	-30.27	-12.80	66.48	15.00
17 LYS CB	-29.26	-13.70	67.22	15.00
17 LYS CG	-29.85	-14.45	68.41	15.00
17 LYS CD	-30.15	-13.52	69.56	15.00
17 LYS CE	-31.10	-14.14	70.58	15.00
17 LYS NZ	-30.73	-15.52	70.94	15.00
17 LYS C	-29.70	-12.43	65.09	15.00
17 LYS O	-30.25	-12.81	64.05	15.00
18 ASN N	-28.59	-11.71	65.10	15.00
18 ASN CA	-27.93	-11.24	63.89	15.00
18 ASN CB	-28.25	-9.75	63.69	15.00
18 ASN CG	-27.74	-9.21	62.37	15.00
18 ASN OD1	-27.34	-9.95	61.49	15.00
18 ASN ND2	-27.75	-7.90	62.24	15.00
18 ASN C	-26.41	-11.47	63.99	15.00
18 ASN O	-25.70	-10.74	64.68	15.00
19 GLN N	-25.92	-12.47	63.27	15.00
19 GLN CA	-24.50	-12.81	63.27	15.00
19 GLN CB	-24.23	-14.05	62.39	15.00
19 GLN CG	-24.59	-13.91	60.91	15.00
19 GLN CD	-24.31	-15.17	60.10	15.00
19 GLN OE1	-25.15	-16.06	60.00	15.00
19 GLN NE2	-23.13	-15.23	59.50	15.00
19 GLN C	-23.59	-11.65	62.84	15.00
19 GLN O	-22.45	-11.56	63.30	15.00
20 GLY N	-24.09	-10.77	61.99	15.00
20 GLY CA	-23.28	-9.65	61.53	15.00
20 GLY C	-22.31	-10.07	60.45	15.00
20 GLY O	-22.59	-10.98	59.67	15.00
21 GLN N	-21.15	-9.43	60.41	15.00
21 GLN CA	-20.14	-9.75	59.41	15.00
21 GLN CB	-19.40	-8.48	58.96	15.00
21 GLN CG	-20.22	-7.59	58.06	15.00
21 GLN CD	-20.48	-8.23	56.69	15.00
21 GLN OE1	-19.88	-9.26	56.33	15.00
21 GLN NE2	-21.37	-7.60	55.90	15.00
21 GLN C	-19.15	-10.78	59.98	15.00

TABLE IV

21 GLN O	-17.95	-10.51	60.13	15.00
22 CYS N	-19.68	-11.95	60.30	15.00
22 CYS CA	-18.90	-13.04	60.86	15.00
22 CYS C	-19.59	-14.32	60.46	15.00
22 CYS O	-20.82	-14.40	60.50	15.00
22 CYS CB	-18.83	-12.90	62.40	15.00
22 CYS SG	-18.13	-14.32	63.33	15.00
23 GLY N	-18.81	-15.30	60.03	15.00
23 GLY CA	-19.36	-16.58	59.63	15.00
23 GLY C	-19.61	-17.48	60.83	15.00
23 GLY O	-19.23	-18.65	60.84	15.00
24 SER N	-20.32	-16.94	61.82	15.00
24 SER CA	-20.63	-17.67	63.03	15.00
24 SER CB	-20.58	-16.71	64.22	15.00
24 SER OG	-21.38	-15.58	64.00	15.00
24 SER C	-22.00	-18.34	62.98	15.00
24 SER O	-22.52	-18.78	64.01	15.00
25 CYS N	-22.59	-18.45	61.79	15.00
25 CYS CA	-23.90	-19.08	61.65	15.00
25 CYS CB	-24.31	-19.15	60.17	15.00
25 CYS SG	-23.12	-20.00	59.06	15.00
25 CYS C	-23.95	-20.47	62.29	15.00
25 CYS O	-24.95	-20.85	62.89	15.00
25 INH C1	-28.28	-9.31	55.94	15.00
25 INH C2	-28.07	-9.03	57.30	15.00
25 INH C3	-27.11	-9.78	58.03	15.00
25 INH C4	-26.37	-10.78	57.40	15.00
25 INH C5	-26.59	-11.05	56.05	15.00
25 INH C6	-27.54	-10.32	55.31	15.00
25 INH C7	-25.31	-11.54	58.16	15.00
25 INH O8	-24.19	-11.68	57.24	15.00
25 INH C9	-23.29	-12.79	57.20	15.00
25 INH O10	-22.50	-12.99	58.13	15.00
25 INH C11	-22.45	-14.71	55.88	15.00
25 INH C12	-21.05	-14.47	56.48	15.00
25 INH C13	-20.11	-13.38	55.92	15.00
25 INH C14	-19.15	-12.91	57.01	15.00
25 INH C15	-20.83	-12.17	55.23	15.00
25 INH C16	-23.00	-16.06	56.34	15.00
25 INH O17	-24.16	-16.15	56.75	15.00
25 INH N18	-22.19	-17.17	56.30	15.00
25 INH N19	-22.62	-18.53	56.74	15.00
25 INH N20	-23.34	-13.55	56.10	15.00

TABLE IV

25 INH C21	-22.09	-18.85	58.14	15.00
25 INH O22	-22.10	-17.80	58.75	15.00
25 INH C23	-12.78	-27.30	59.77	15.00
25 INH C24	-13.75	-26.80	60.62	15.00
25 INH C25	-14.61	-25.79	60.17	15.00
25 INH C26	-14.52	-25.29	58.88	15.00
25 INH C27	-13.54	-25.80	58.03	15.00
25 INH C28	-12.67	-26.81	58.47	15.00
25 INH C29	-15.45	-24.21	58.40	15.00
25 INH O30	-16.52	-24.58	57.49	15.00
25 INH C31	-17.56	-23.66	57.05	15.00
25 INH O32	-17.32	-22.74	56.27	15.00
25 INH C33	-19.95	-23.09	57.18	15.00
25 INH C34	-21.23	-23.90	57.35	15.00
25 INH C35	-21.11	-25.25	58.03	15.00
25 INH C36	-22.32	-25.59	58.89	15.00
25 INH C37	-20.84	-26.31	56.99	15.00
25 INH C38	-20.07	-21.83	58.03	15.00
25 INH O39	-19.74	-21.86	59.22	15.00
25 INH N40	-20.56	-20.70	57.43	15.00
25 INH N41	-20.70	-19.44	58.21	15.00
25 INH N42	-18.78	-23.90	57.54	15.00
26 TRP N	-22.83	-21.19	62.21	15.00
26 TRP CA	-22.70	-22.53	62.79	15.00
26 TRP CB	-21.33	-23.13	62.41	15.00
26 TRP CG	-20.12	-22.32	62.88	15.00
26 TRP CD2	-19.43	-22.44	64.14	15.00
26 TRP CE2	-18.42	-21.46	64.16	15.00
26 TRP CE3	-19.58	-23.27	65.26	15.00
26 TRP CD1	-19.50	-21.31	62.20	15.00
26 TRP NE1	-18.48	-20.79	62.96	15.00
26 TRP CZ2	-17.56	-21.29	65.25	15.00
26 TRP CZ3	-18.73	-23.10	66.34	15.00
26 TRP CH2	-17.73	-22.11	66.33	15.00
26 TRP C	-22.87	-22.47	64.31	15.00
26 TRP O	-23.46	-23.36	64.91	15.00
27 ALA N	-22.37	-21.39	64.90	15.00
27 ALA CA	-22.43	-21.17	66.34	15.00
27 ALA CB	-21.53	-20.00	66.72	15.00
27 ALA C	-23.87	-20.90	66.77	15.00
27 ALA O	-24.34	-21.42	67.78	15.00
28 PHE N	-24.55	-20.06	65.99	15.00
28 PHE CA	-25.94	-19.71	66.23	15.00

TABLE IV

28 PHE CB	-26.38	-18.58	65.29	15.00
28 PHE CG	-25.85	-17.23	65.70	15.00
28 PHE CD1	-24.59	-16.81	65.30	15.00
28 PHE CD2	-26.60	-16.39	66.52	15.00
28 PHE CE1	-24.08	-15.57	65.70	15.00
28 PHE CE2	-26.09	-15.15	66.93	15.00
28 PHE CZ	-24.83	-14.74	66.52	15.00
28 PHE C	-26.86	-20.93	66.07	15.00
28 PHE O	-27.82	-21.10	66.82	15.00
29 SER N	-26.54	-21.81	65.13	15.00
29 SER CA	-27.33	-23.01	64.93	15.00
29 SER CB	-26.85	-23.73	63.66	15.00
29 SER OG	-27.55	-24.93	63.47	15.00
29 SER C	-27.19	-23.93	66.16	15.00
29 SER O	-28.19	-24.39	66.71	15.00
30 SER N	-25.95	-24.16	66.59	15.00
30 SER CA	-25.63	-25.00	67.75	15.00
30 SER CB	-24.12	-24.97	68.04	15.00
30 SER OG	-23.34	-25.28	66.91	15.00
30 SER C	-26.36	-24.51	68.98	15.00
30 SER O	-27.02	-25.26	69.69	15.00
31 VAL N	-26.16	-23.23	69.26	15.00
31 VAL CA	-26.76	-22.55	70.39	15.00
31 VAL CB	-26.31	-21.07	70.38	15.00
31 VAL CG1	-27.42	-20.13	70.84	15.00
31 VAL CG2	-25.08	-20.92	71.26	15.00
31 VAL C	-28.28	-22.70	70.37	15.00
31 VAL O	-28.87	-23.11	71.37	15.00
32 GLY N	-28.89	-22.44	69.22	15.00
32 GLY CA	-30.32	-22.56	69.08	15.00
32 GLY C	-30.79	-23.96	69.45	15.00
32 GLY O	-31.80	-24.12	70.14	15.00
33 ALA N	-30.03	-24.96	69.01	15.00
33 ALA CA	-30.35	-26.35	69.30	15.00
33 ALA CB	-29.44	-27.29	68.48	15.00
33 ALA C	-30.24	-26.64	70.80	15.00
33 ALA O	-31.11	-27.29	71.38	15.00
34 LEU N	-29.17	-26.15	71.42	15.00
34 LEU CA	-28.96	-26.37	72.84	15.00
34 LEU CB	-27.61	-25.82	73.28	15.00
34 LEU CG	-26.39	-26.66	72.87	15.00
34 LEU CD1	-25.12	-25.82	72.89	15.00
34 LEU CD2	-26.27	-27.87	73.78	15.00

TABLE IV

34 LEU C	-30.09	-25.73	73.66	15.00
34 LEU O	-30.62	-26.34	74.59	15.00
35 GLU N	-30.48	-24.53	73.25	15.00
35 GLU CA	-31.55	-23.78	73.90	15.00
35 GLU CB	-31.70	-22.41	73.25	15.00
35 GLU CG	-30.49	-21.53	73.41	15.00
35 GLU CD	-30.59	-20.25	72.60	15.00
35 GLU OE1	-31.42	-20.17	71.67	15.00
35 GLU OE2	-29.81	-19.32	72.90	15.00
35 GLU C	-32.89	-24.52	73.87	15.00
35 GLU O	-33.66	-24.41	74.81	15.00
36 GLY N	-33.16	-25.25	72.79	15.00
36 GLY CA	-34.41	-25.97	72.72	15.00
36 GLY C	-34.42	-27.05	73.78	15.00
36 GLY O	-35.32	-27.13	74.61	15.00
37 GLN N	-33.35	-27.86	73.77	15.00
37 GLN CA	-33.18	-28.95	74.71	15.00
37 GLN CB	-31.95	-29.77	74.32	15.00
37 GLN CG	-32.01	-30.34	72.91	15.00
37 GLN CD	-33.22	-31.25	72.69	15.00
37 GLN OE1	-33.31	-32.35	73.26	15.00
37 GLN NE2	-34.16	-30.78	71.87	15.00
37 GLN C	-33.10	-28.48	76.17	15.00
37 GLN O	-33.70	-29.09	77.06	15.00
38 LEU N	-32.38	-27.39	76.40	15.00
38 LEU CA	-32.27	-26.87	77.75	15.00
38 LEU CB	-31.39	-25.63	77.79	15.00
38 LEU CG	-31.34	-25.01	79.18	15.00
38 LEU CD1	-30.49	-25.87	80.11	15.00
38 LEU CD2	-30.79	-23.61	79.08	15.00
38 LEU C	-33.65	-26.51	78.26	15.00
38 LEU O	-33.97	-26.73	79.43	15.00
39 LYS N	-34.45	-25.90	77.38	15.00
39 LYS CA	-35.81	-25.51	77.72	15.00
39 LYS CB	-36.42	-24.72	76.55	15.00
39 LYS CG	-37.63	-23.88	76.91	15.00
39 LYS CD	-38.88	-24.71	77.08	15.00
39 LYS CE	-39.79	-24.14	78.15	15.00
39 LYS NZ	-39.99	-22.66	78.01	15.00
39 LYS C	-36.61	-26.78	78.00	15.00
39 LYS O	-37.28	-26.89	79.04	15.00
40 LYS N	-36.48	-27.75	77.11	15.00
40 LYS CA	-37.19	-29.01	77.23	15.00

TABLE IV

40 LYS CB	-36.93	-29.90	76.01	15.00
40 LYS CG	-37.84	-31.13	75.91	15.00
40 LYS CD	-37.59	-31.87	74.60	15.00
40 LYS CE	-37.06	-33.28	74.85	15.00
40 LYS NZ	-36.36	-33.87	73.66	15.00
40 LYS C	-36.82	-29.76	78.51	15.00
40 LYS O	-37.69	-30.36	79.16	15.00
41 LYS N	-35.55	-29.66	78.92	15.00
41 LYS CA	-35.08	-30.37	80.10	15.00
41 LYS CB	-33.60	-30.71	79.95	15.00
41 LYS CG	-33.12	-31.74	80.95	15.00
41 LYS CD	-31.66	-32.10	80.76	15.00
41 LYS CE	-31.18	-33.02	81.87	15.00
41 LYS NZ	-31.86	-34.35	81.80	15.00
41 LYS C	-35.32	-29.68	81.45	15.00
41 LYS O	-35.76	-30.32	82.40	15.00
42 THR N	-35.04	-28.38	81.51	15.00
42 THR CA	-35.19	-27.62	82.75	15.00
42 THR CB	-34.00	-26.66	82.95	15.00
42 THR OG1	-34.10	-25.58	82.01	15.00
42 THR CG2	-32.68	-27.39	82.71	15.00
42 THR C	-36.46	-26.78	82.86	15.00
42 THR O	-36.86	-26.41	83.96	15.00
43 GLY N	-37.04	-26.42	81.73	15.00
43 GLY CA	-38.24	-25.60	81.75	15.00
43 GLY C	-37.95	-24.12	81.59	15.00
43 GLY O	-38.88	-23.31	81.62	15.00
44 LYS N	-36.67	-23.75	81.48	15.00
44 LYS CA	-36.28	-22.35	81.31	15.00
44 LYS CB	-35.14	-21.96	82.26	15.00
44 LYS CG	-35.58	-21.64	83.67	15.00
44 LYS CD	-35.80	-22.90	84.47	15.00
44 LYS CE	-34.48	-23.49	84.91	15.00
44 LYS NZ	-33.81	-22.59	85.90	15.00
44 LYS C	-35.82	-22.07	79.87	15.00
44 LYS O	-35.33	-22.95	79.19	15.00
45 LEU N	-35.97	-20.82	79.44	15.00
45 LEU CA	-35.56	-20.40	78.11	15.00
45 LEU CB	-36.79	-20.00	77.26	15.00
45 LEU CG	-36.54	-19.61	75.80	15.00
45 LEU CD1	-36.32	-20.88	74.98	15.00
45 LEU CD2	-37.71	-18.81	75.22	15.00
45 LEU C	-34.65	-19.18	78.26	15.00

TABLE IV

45 LEU O	-35.09	-18.11	78.69	15.00
46 LEU N	-33.36	-19.38	78.00	15.00
46 LEU CA	-32.41	-18.30	78.06	15.00
46 LEU CB	-31.64	-18.25	79.40	15.00
46 LEU CG	-30.80	-19.34	80.08	15.00
46 LEU CD1	-31.61	-20.01	81.15	15.00
46 LEU CD2	-30.27	-20.35	79.09	15.00
46 LEU C	-31.46	-18.38	76.86	15.00
46 LEU O	-31.39	-19.40	76.17	15.00
47 ASN N	-30.79	-17.27	76.59	15.00
47 ASN CA	-29.86	-17.18	75.47	15.00
47 ASN CB	-29.74	-15.73	75.04	15.00
47 ASN CG	-31.07	-15.14	74.66	15.00
47 ASN OD1	-31.74	-15.64	73.75	15.00
47 ASN ND2	-31.50	-14.13	75.39	15.00
47 ASN C	-28.51	-17.75	75.81	15.00
47 ASN O	-27.91	-17.37	76.81	15.00
48 LEU N	-28.07	-18.74	75.05	15.00
48 LEU CA	-26.77	-19.34	75.27	15.00
48 LEU CB	-26.81	-20.84	74.95	15.00
48 LEU CG	-27.74	-21.60	75.90	15.00
48 LEU CD1	-27.67	-23.09	75.67	15.00
48 LEU CD2	-27.37	-21.30	77.33	15.00
48 LEU C	-25.77	-18.57	74.42	15.00
48 LEU O	-26.17	-17.88	73.47	15.00
49 SER N	-24.50	-18.67	74.76	15.00
49 SER CA	-23.45	-17.92	74.09	15.00
49 SER CB	-22.32	-17.62	75.08	15.00
49 SER OG	-21.28	-16.87	74.48	15.00
49 SER C	-22.83	-18.44	72.80	15.00
49 SER O	-22.08	-19.40	72.82	15.00
50 PRO N	-23.10	-17.78	71.67	15.00
50 PRO CD	-24.13	-16.75	71.42	15.00
50 PRO CA	-22.50	-18.23	70.41	15.00
50 PRO CB	-23.27	-17.43	69.35	15.00
50 PRO CG	-24.58	-17.10	70.04	15.00
50 PRO C	-21.01	-17.85	70.42	15.00
50 PRO O	-20.16	-18.58	69.92	15.00
51 GLN N	-20.70	-16.70	71.03	15.00
51 GLN CA	-19.34	-16.20	71.12	15.00
51 GLN CB	-19.32	-14.84	71.83	15.00
51 GLN CG	-18.00	-14.10	71.73	15.00
51 GLN CD	-17.72	-13.59	70.34	15.00

TABLE IV

51	GLN	OE1	-18.55	-12.90	69.73	15.00
51	GLN	NE2	-16.55	-13.90	69.82	15.00
51	GLN	C	-18.45	-17.21	71.86	15.00
51	GLN	O	-17.28	-17.39	71.50	15.00
52	ASN	N	-19.01	-17.87	72.87	15.00
52	ASN	CA	-18.28	-18.88	73.62	15.00
52	ASN	CB	-19.24	-19.57	74.60	15.00
52	ASN	CG	-18.54	-20.47	75.63	15.00
52	ASN	OD1	-19.19	-20.95	76.57	15.00
52	ASN	ND2	-17.24	-20.70	75.48	15.00
52	ASN	C	-17.74	-19.88	72.59	15.00
52	ASN	O	-16.55	-20.22	72.60	15.00
53	LEU	N	-18.60	-20.31	71.68	15.00
53	LEU	CA	-18.22	-21.26	70.64	15.00
53	LEU	CB	-19.47	-21.70	69.86	15.00
53	LEU	CG	-20.37	-22.81	70.42	15.00
53	LEU	CD1	-20.05	-23.13	71.87	15.00
53	LEU	CD2	-21.83	-22.41	70.22	15.00
53	LEU	C	-17.18	-20.69	69.68	15.00
53	LEU	O	-16.17	-21.33	69.40	15.00
54	VAL	N	-17.44	-19.48	69.18	15.00
54	VAL	CA	-16.55	-18.82	68.23	15.00
54	VAL	CB	-17.03	-17.36	67.92	15.00
54	VAL	CG1	-15.96	-16.58	67.19	15.00
54	VAL	CG2	-18.28	-17.40	67.05	15.00
54	VAL	C	-15.10	-18.79	68.72	15.00
54	VAL	O	-14.19	-19.17	67.98	15.00
55	ASP	N	-14.90	-18.37	69.96	15.00
55	ASP	CA	-13.56	-18.26	70.51	15.00
55	ASP	CB	-13.56	-17.25	71.67	15.00
55	ASP	CG	-14.04	-15.87	71.27	15.00
55	ASP	OD1	-14.02	-15.54	70.06	15.00
55	ASP	OD2	-14.43	-15.10	72.18	15.00
55	ASP	C	-12.93	-19.55	71.04	15.00
55	ASP	O	-11.72	-19.70	71.00	15.00
56	CYS	N	-13.76	-20.47	71.50	15.00
56	CYS	CA	-13.26	-21.69	72.14	15.00
56	CYS	C	-13.18	-23.02	71.37	15.00
56	CYS	O	-12.34	-23.86	71.72	15.00
56	CYS	CB	-14.03	-21.89	73.45	15.00
56	CYS	SG	-14.05	-20.41	74.53	15.00
57	VAL	N	-14.03	-23.22	70.37	15.00
57	VAL	CA	-14.00	-24.47	69.62	15.00

TABLE IV

57 VAL CB	-15.34	-24.76	68.86	15.00
57 VAL CG1	-15.38	-26.20	68.38	15.00
57 VAL CG2	-16.52	-24.51	69.77	15.00
57 VAL C	-12.80	-24.45	68.66	15.00
57 VAL O	-12.85	-23.83	67.60	15.00
58 SER N	-11.72	-25.10	69.08	15.00
58 SER CA	-10.48	-25.16	68.32	15.00
58 SER CB	-9.34	-25.68	69.21	15.00
58 SER OG	-9.70	-26.91	69.82	15.00
58 SER C	-10.53	-25.97	67.03	15.00
58 SER O	-9.67	-25.81	66.17	15.00
59 GLU N	-11.49	-26.88	66.92	15.00
59 GLU CA	-11.62	-27.68	65.70	15.00
59 GLU CB	-12.33	-29.00	65.99	15.00
59 GLU CG	-11.57	-29.96	66.92	15.00
59 GLU CD	-11.66	-29.59	68.40	15.00
59 GLU OE1	-10.69	-29.88	69.12	15.00
59 GLU OE2	-12.69	-29.03	68.85	15.00
59 GLU C	-12.37	-26.89	64.62	15.00
59 GLU O	-12.48	-27.34	63.49	15.00
60 ASN N	-12.91	-25.73	64.98	15.00
60 ASN CA	-13.65	-24.87	64.06	15.00
60 ASN CB	-14.99	-24.44	64.66	15.00
60 ASN CG	-16.08	-25.51	64.51	15.00
60 ASN OD1	-17.16	-25.38	65.08	15.00
60 ASN ND2	-15.79	-26.55	63.74	15.00
60 ASN C	-12.81	-23.65	63.73	15.00
60 ASN O	-11.76	-23.44	64.35	15.00
61 ASP N	-13.28	-22.85	62.78	15.00
61 ASP CA	-12.53	-21.67	62.38	15.00
61 ASP CB	-12.22	-21.74	60.88	15.00
61 ASP CG	-11.54	-23.04	60.50	15.00
61 ASP OD1	-12.02	-23.72	59.56	15.00
61 ASP OD2	-10.54	-23.41	61.16	15.00
61 ASP C	-13.13	-20.31	62.74	15.00
61 ASP O	-12.89	-19.32	62.04	15.00
62 GLY N	-13.88	-20.27	63.83	15.00
62 GLY CA	-14.48	-19.03	64.30	15.00
62 GLY C	-15.34	-18.30	63.30	15.00
62 GLY O	-16.37	-18.81	62.87	15.00
63 CYS N	-14.96	-17.07	62.96	15.00
63 CYS CA	-15.71	-16.28	61.99	15.00
63 CYS C	-15.49	-16.79	60.56	15.00

TABLE IV

63	CYS	O	-16.19	-16.39	59.63	15.00
63	CYS	CB	-15.37	-14.79	62.10	15.00
63	CYS	SG	-16.14	-13.94	63.53	15.00
64	GLY	N	-14.55	-17.71	60.41	15.00
64	GLY	CA	-14.27	-18.27	59.10	15.00
64	GLY	C	-15.11	-19.50	58.79	15.00
64	GLY	O	-14.95	-20.10	57.73	15.00
65	GLY	N	-15.94	-19.92	59.74	15.00
65	GLY	CA	-16.78	-21.08	59.52	15.00
65	GLY	C	-16.54	-22.20	60.51	15.00
65	GLY	O	-15.54	-22.20	61.24	15.00
66	GLY	N	-17.44	-23.18	60.52	15.00
66	GLY	CA	-17.29	-24.31	61.41	15.00
66	GLY	C	-18.41	-25.32	61.27	15.00
66	GLY	O	-19.25	-25.19	60.37	15.00
67	TYR	N	-18.41	-26.34	62.13	15.00
67	TYR	CA	-19.42	-27.39	62.15	15.00
67	TYR	CB	-18.78	-28.74	61.83	15.00
67	TYR	CG	-18.30	-28.84	60.41	15.00
67	TYR	CD1	-19.02	-29.55	59.47	15.00
67	TYR	CE1	-18.62	-29.59	58.13	15.00
67	TYR	CD2	-17.15	-28.16	60.00	15.00
67	TYR	CE2	-16.74	-28.19	58.67	15.00
67	TYR	CZ	-17.48	-28.90	57.74	15.00
67	TYR	OH	-17.12	-28.88	56.42	15.00
67	TYR	C	-20.12	-27.46	63.51	15.00
67	TYR	O	-19.48	-27.31	64.54	15.00
68	MET	N	-21.43	-27.73	63.50	15.00
68	MET	CA	-22.22	-27.81	64.73	15.00
68	MET	CB	-23.72	-27.83	64.41	15.00
68	MET	CG	-24.26	-26.60	63.63	15.00
68	MET	SD	-24.05	-26.62	61.79	15.00
68	MET	CE	-25.42	-27.66	61.31	15.00
68	MET	C	-21.84	-29.02	65.61	15.00
68	MET	O	-21.89	-28.95	66.84	15.00
69	THR	N	-21.48	-30.12	64.98	15.00
69	THR	CA	-21.08	-31.33	65.70	15.00
69	THR	CB	-20.80	-32.51	64.73	15.00
69	THR	OG1	-20.08	-32.02	63.58	15.00
69	THR	CG2	-22.12	-33.15	64.27	15.00
69	THR	C	-19.82	-31.05	66.53	15.00
69	THR	O	-19.67	-31.55	67.66	15.00
70	ASN	N	-18.94	-30.21	65.99	15.00

TABLE IV

70 ASN CA	-17.72	-29.85	66.69	15.00
70 ASN CB	-16.76	-29.07	65.79	15.00
70 ASN CG	-15.89	-29.97	64.95	15.00
70 ASN OD1	-15.35	-29.56	63.93	15.00
70 ASN ND2	-15.72	-31.21	65.39	15.00
70 ASN C	-18.08	-29.02	67.91	15.00
70 ASN O	-17.57	-29.25	69.00	15.00
71 ALA N	-19.02	-28.09	67.71	15.00
71 ALA CA	-19.50	-27.22	68.77	15.00
71 ALA CB	-20.49	-26.20	68.21	15.00
71 ALA C	-20.14	-28.02	69.90	15.00
71 ALA O	-19.88	-27.76	71.07	15.00
72 PHE N	-20.90	-29.05	69.55	15.00
72 PHE CA	-21.56	-29.89	70.55	15.00
72 PHE CB	-22.55	-30.86	69.89	15.00
72 PHE CG	-23.72	-30.18	69.24	15.00
72 PHE CD1	-24.30	-29.05	69.82	15.00
72 PHE CD2	-24.23	-30.65	68.04	15.00
72 PHE CE1	-25.38	-28.41	69.21	15.00
72 PHE CE2	-25.31	-30.01	67.42	15.00
72 PHE CZ	-25.89	-28.89	68.01	15.00
72 PHE C	-20.53	-30.68	71.37	15.00
72 PHE O	-20.66	-30.76	72.60	15.00
73 GLN N	-19.55	-31.27	70.69	15.00
73 GLN CA	-18.50	-32.05	71.34	15.00
73 GLN CB	-17.52	-32.66	70.34	15.00
73 GLN CG	-18.09	-33.80	69.51	15.00
73 GLN CD	-17.03	-34.63	68.79	15.00
73 GLN OE1	-17.20	-35.01	67.62	15.00
73 GLN NE2	-15.95	-34.94	69.49	15.00
73 GLN C	-17.75	-31.16	72.30	15.00
73 GLN O	-17.35	-31.61	73.38	15.00
74 TYR N	-17.55	-29.89	71.92	15.00
74 TYR CA	-16.84	-28.94	72.75	15.00
74 TYR CB	-16.75	-27.57	72.08	15.00
74 TYR CG	-16.46	-26.43	73.03	15.00
74 TYR CD1	-15.18	-26.26	73.58	15.00
74 TYR CE1	-14.91	-25.23	74.50	15.00
74 TYR CD2	-17.46	-25.54	73.42	15.00
74 TYR CE2	-17.21	-24.51	74.34	15.00
74 TYR CZ	-15.93	-24.36	74.88	15.00
74 TYR OH	-15.69	-23.36	75.78	15.00
74 TYR C	-17.58	-28.81	74.06	15.00

TABLE IV

74 TYR O	-17.02	-29.09	75.12	15.00
75 VAL N	-18.84	-28.39	73.99	15.00
75 VAL CA	-19.67	-28.21	75.17	15.00
75 VAL CB	-21.14	-27.89	74.77	15.00
75 VAL CG1	-22.00	-27.77	76.01	15.00
75 VAL CG2	-21.20	-26.59	73.96	15.00
75 VAL C	-19.61	-29.43	76.09	15.00
75 VAL O	-19.55	-29.27	77.31	15.00
76 GLN N	-19.56	-30.63	75.51	15.00
76 GLN CA	-19.48	-31.85	76.29	15.00
76 GLN CB	-19.68	-33.09	75.42	15.00
76 GLN CG	-19.53	-34.39	76.19	15.00
76 GLN CD	-19.73	-35.63	75.35	15.00
76 GLN OE1	-19.39	-35.66	74.17	15.00
76 GLN NE2	-20.27	-36.67	75.97	15.00
76 GLN C	-18.15	-31.96	77.03	15.00
76 GLN O	-18.14	-32.20	78.23	15.00
77 LYS N	-17.05	-31.81	76.30	15.00
77 LYS CA	-15.70	-31.90	76.87	15.00
77 LYS CB	-14.63	-31.71	75.79	15.00
77 LYS CG	-14.73	-32.63	74.61	15.00
77 LYS CD	-14.44	-34.07	74.97	15.00
77 LYS CE	-14.49	-34.96	73.73	15.00
77 LYS NZ	-13.56	-34.52	72.63	15.00
77 LYS C	-15.51	-30.80	77.93	15.00
77 LYS O	-15.07	-31.05	79.04	15.00
78 ASN N	-15.87	-29.58	77.55	15.00
78 ASN CA	-15.78	-28.42	78.42	15.00
78 ASN CB	-16.11	-27.17	77.61	15.00
78 ASN CG	-15.75	-25.90	78.33	15.00
78 ASN OD1	-14.65	-25.77	78.86	15.00
78 ASN ND2	-16.66	-24.93	78.33	15.00
78 ASN C	-16.76	-28.55	79.61	15.00
78 ASN O	-16.66	-27.82	80.59	15.00
79 ARG N	-17.70	-29.48	79.47	15.00
79 ARG CA	-18.73	-29.76	80.46	15.00
79 ARG CB	-18.11	-30.22	81.77	15.00
79 ARG CG	-17.42	-31.56	81.70	15.00
79 ARG CD	-16.95	-31.93	83.08	15.00
79 ARG NE	-16.17	-33.15	83.11	15.00
79 ARG CZ	-14.86	-33.22	82.89	15.00
79 ARG NH1	-14.17	-32.13	82.58	15.00
79 ARG NH2	-14.21	-34.37	83.07	15.00

TABLE IV

79 ARG C	-19.66	-28.58	80.71	15.00
79 ARG O	-20.27	-28.49	81.78	15.00
80 GLY N	-19.79	-27.70	79.72	15.00
80 GLY CA	-20.65	-26.55	79.87	15.00
80 GLY C	-20.48	-25.48	78.81	15.00
80 GLY O	-19.54	-25.52	78.01	15.00
81 ILE N	-21.41	-24.53	78.80	15.00
81 ILE CA	-21.40	-23.40	77.88	15.00
81 ILE CB	-22.23	-23.68	76.58	15.00
81 ILE CG2	-23.68	-24.05	76.93	15.00
81 ILE CG1	-22.19	-22.46	75.64	15.00
81 ILE CD1	-22.89	-22.66	74.31	15.00
81 ILE C	-21.99	-22.20	78.62	15.00
81 ILE O	-22.91	-22.35	79.43	15.00
82 ASP N	-21.44	-21.02	78.37	15.00
82 ASP CA	-21.91	-19.81	79.01	15.00
82 ASP CB	-20.85	-18.71	78.94	15.00
82 ASP CG	-19.73	-18.92	79.95	15.00
82 ASP OD1	-18.66	-18.32	79.78	15.00
82 ASP OD2	-19.93	-19.69	80.91	15.00
82 ASP C	-23.21	-19.25	78.45	15.00
82 ASP O	-23.63	-19.58	77.33	15.00
83 SER N	-23.86	-18.43	79.26	15.00
83 SER CA	-25.09	-17.78	78.85	15.00
83 SER CB	-25.92	-17.36	80.08	15.00
83 SER OG	-25.25	-16.38	80.86	15.00
83 SER C	-24.65	-16.55	78.06	15.00
83 SER O	-23.50	-16.10	78.17	15.00
84 GLU N	-25.56	-16.01	77.26	15.00
84 GLU CA	-25.27	-14.83	76.47	15.00
84 GLU CB	-26.53	-14.40	75.70	15.00
84 GLU CG	-26.39	-13.10	74.93	15.00
84 GLU CD	-25.30	-13.12	73.85	15.00
84 GLU OE1	-24.76	-12.04	73.52	15.00
84 GLU OE2	-24.98	-14.22	73.33	15.00
84 GLU C	-24.77	-13.70	77.38	15.00
84 GLU O	-23.77	-13.09	77.06	15.00
85 ASP N	-25.44	-13.47	78.51	15.00
85 ASP CA	-25.05	-12.41	79.46	15.00
85 ASP CB	-26.03	-12.35	80.65	15.00
85 ASP CG	-27.20	-11.39	80.42	15.00
85 ASP OD1	-27.86	-11.50	79.37	15.00
85 ASP OD2	-27.47	-10.53	81.29	15.00

TABLE IV

85 ASP C	-23.62	-12.54	79.98	15.00
85 ASP O	-22.89	-11.55	80.07	15.00
86 ALA N	-23.23	-13.77	80.27	15.00
86 ALA CA	-21.91	-14.09	80.78	15.00
86 ALA CB	-21.95	-15.45	81.49	15.00
86 ALA C	-20.79	-14.09	79.71	15.00
86 ALA O	-19.61	-14.21	80.04	15.00
87 TYR N	-21.16	-13.98	78.44	15.00
87 TYR CA	-20.18	-13.99	77.36	15.00
87 TYR CB	-19.75	-15.44	77.09	15.00
87 TYR CG	-18.36	-15.67	76.52	15.00
87 TYR CD1	-17.82	-14.83	75.54	15.00
87 TYR CE1	-16.55	-15.09	74.99	15.00
87 TYR CD2	-17.60	-16.76	76.94	15.00
87 TYR CE2	-16.34	-17.03	76.40	15.00
87 TYR CZ	-15.82	-16.19	75.42	15.00
87 TYR OH	-14.59	-16.49	74.88	15.00
87 TYR C	-20.90	-13.42	76.14	15.00
87 TYR O	-21.25	-14.15	75.22	15.00
88 PRO N	-21.09	-12.09	76.11	15.00
88 PRO CD	-20.58	-11.10	77.08	15.00
88 PRO CA	-21.77	-11.42	75.00	15.00
88 PRO CB	-21.83	-9.97	75.47	15.00
88 PRO CG	-20.62	-9.82	76.28	15.00
88 PRO C	-21.13	-11.58	73.62	15.00
88 PRO O	-19.92	-11.77	73.47	15.00
89 TYR N	-21.98	-11.45	72.61	15.00
89 TYR CA	-21.56	-11.59	71.22	15.00
89 TYR CB	-22.77	-11.93	70.35	15.00
89 TYR CG	-22.41	-12.26	68.92	15.00
89 TYR CD1	-21.67	-13.41	68.62	15.00
89 TYR CE1	-21.30	-13.71	67.32	15.00
89 TYR CD2	-22.78	-11.43	67.87	15.00
89 TYR CE2	-22.41	-11.72	66.56	15.00
89 TYR CZ	-21.68	-12.87	66.30	15.00
89 TYR OH	-21.29	-13.15	65.01	15.00
89 TYR C	-20.91	-10.31	70.72	15.00
89 TYR O	-21.45	-9.21	70.89	15.00
90 VAL N	-19.73	-10.45	70.13	15.00
90 VAL CA	-19.01	-9.31	69.58	15.00
90 VAL CB	-17.59	-9.14	70.23	15.00
90 VAL CG1	-17.71	-8.96	71.73	15.00
90 VAL CG2	-16.69	-10.31	69.89	15.00

TABLE IV

90 VAL C	-18.88	-9.45	68.06	15.00
90 VAL O	-18.50	-8.50	67.38	15.00
91 GLY N	-19.17	-10.63	67.53	15.00
91 GLY CA	-19.08	-10.82	66.09	15.00
91 GLY C	-17.67	-10.74	65.55	15.00
91 GLY O	-17.44	-10.33	64.40	15.00
92 GLN N	-16.71	-11.14	66.37	15.00
92 GLN CA	-15.31	-11.12	66.00	15.00
92 GLN CB	-14.73	-9.72	66.26	15.00
92 GLN CG	-13.35	-9.49	65.65	15.00
92 GLN CD	-12.71	-8.19	66.08	15.00
92 GLN OE1	-12.20	-7.44	65.24	15.00
92 GLN NE2	-12.73	-7.92	67.39	15.00
92 GLN C	-14.60	-12.19	66.82	15.00
92 GLN O	-15.02	-12.50	67.94	15.00
93 GLU N	-13.54	-12.78	66.26	15.00
93 GLU CA	-12.77	-13.82	66.94	15.00
93 GLU CB	-11.86	-14.56	65.94	15.00
93 GLU CG	-12.59	-15.03	64.68	15.00
93 GLU CD	-11.65	-15.50	63.57	15.00
93 GLU OE1	-10.57	-14.88	63.36	15.00
93 GLU OE2	-12.02	-16.49	62.88	15.00
93 GLU C	-11.92	-13.20	68.04	15.00
93 GLU O	-11.31	-12.14	67.84	15.00
94 GLU N	-11.90	-13.84	69.20	15.00
94 GLU CA	-11.15	-13.38	70.36	15.00
94 GLU CB	-12.03	-12.49	71.25	15.00
94 GLU CG	-12.71	-11.36	70.48	15.00
94 GLU CD	-13.30	-10.28	71.35	15.00
94 GLU OE1	-13.81	-10.60	72.43	15.00
94 GLU OE2	-13.27	-9.10	70.94	15.00
94 GLU C	-10.70	-14.63	71.11	15.00
94 GLU O	-11.13	-15.74	70.77	15.00
95 SER N	-9.82	-14.46	72.10	15.00
95 SER CA	-9.32	-15.60	72.86	15.00
95 SER CB	-8.13	-15.19	73.73	15.00
95 SER OG	-8.46	-14.11	74.58	15.00
95 SER C	-10.40	-16.21	73.74	15.00
95 SER O	-11.26	-15.51	74.26	15.00
96 CYS N	-10.31	-17.52	73.95	15.00
96 CYS CA	-11.30	-18.20	74.78	15.00
96 CYS C	-11.28	-17.68	76.21	15.00
96 CYS O	-10.25	-17.71	76.89	15.00

TABLE IV

96 CYS CB	-11.10	-19.72	74.74	15.00
96 CYS SG	-12.37	-20.66	75.65	15.00
97 MET N	-12.43	-17.18	76.66	15.00
97 MET CA	-12.57	-16.63	77.99	15.00
97 MET CB	-12.71	-15.10	77.90	15.00
97 MET CG	-12.32	-14.33	79.15	15.00
97 MET SD	-10.53	-14.18	79.36	15.00
97 MET CE	-10.23	-15.44	80.61	15.00
97 MET C	-13.83	-17.23	78.62	15.00
97 MET O	-14.71	-16.50	79.08	15.00
98 TYR N	-13.95	-18.55	78.57	15.00
98 TYR CA	-15.11	-19.23	79.14	15.00
98 TYR CB	-15.04	-20.74	78.86	15.00
98 TYR CG	-16.04	-21.57	79.65	15.00
98 TYR CD1	-17.41	-21.44	79.44	15.00
98 TYR CE1	-18.32	-22.23	80.14	15.00
98 TYR CD2	-15.60	-22.52	80.59	15.00
98 TYR CE2	-16.51	-23.31	81.29	15.00
98 TYR CZ	-17.87	-23.16	81.06	15.00
98 TYR OH	-18.78	-23.95	81.71	15.00
98 TYR C	-15.16	-19.00	80.66	15.00
98 TYR O	-14.22	-19.33	81.36	15.00
99 ASN N	-16.23	-18.37	81.13	15.00
99 ASN CA	-16.39	-18.12	82.56	15.00
99 ASN CB	-17.13	-16.81	82.81	15.00
99 ASN CG	-17.36	-16.54	84.30	15.00
99 ASN OD1	-17.39	-17.46	85.12	15.00
99 ASN ND2	-17.54	-15.27	84.65	15.00
99 ASN C	-17.18	-19.27	83.16	15.00
99 ASN O	-18.38	-19.39	82.93	15.00
100 PRO N	-16.53	-20.09	83.98	15.00
100 PRO CD	-15.13	-19.95	84.42	15.00
100 PRO CA	-17.17	-21.24	84.63	15.00
100 PRO CB	-16.08	-21.75	85.57	15.00
100 PRO CG	-14.80	-21.33	84.89	15.00
100 PRO C	-18.43	-20.86	85.40	15.00
100 PRO O	-19.41	-21.59	85.40	15.00
101 THR N	-18.41	-19.69	86.04	15.00
101 THR CA	-19.54	-19.24	86.84	15.00
101 THR CB	-19.09	-18.26	87.95	15.00
101 THR OG1	-18.60	-17.04	87.37	15.00
101 THR CG2	-17.99	-18.90	88.79	15.00
101 THR C	-20.73	-18.68	86.08	15.00

TABLE IV

101 THR O	-21.79	-18.43	86.66	15.00
102 GLY N	-20.57	-18.48	84.77	15.00
102 GLY CA	-21.68	-17.98	83.97	15.00
102 GLY C	-22.30	-19.14	83.21	15.00
102 GLY O	-23.13	-18.94	82.32	15.00
103 LYS N	-21.88	-20.35	83.54	15.00
103 LYS CA	-22.36	-21.57	82.90	15.00
103 LYS CB	-21.73	-22.79	83.58	15.00
103 LYS CG	-22.11	-24.13	82.98	15.00
103 LYS CD	-21.50	-25.25	83.81	15.00
103 LYS CE	-21.82	-25.07	85.28	15.00
103 LYS NZ	-21.22	-26.16	86.10	15.00
103 LYS C	-23.89	-21.67	82.95	15.00
103 LYS O	-24.50	-21.54	84.00	15.00
104 ALA N	-24.50	-21.89	81.79	15.00
104 ALA CA	-25.95	-21.97	81.72	15.00
104 ALA CB	-26.48	-20.90	80.77	15.00
104 ALA C	-26.45	-23.35	81.32	15.00
104 ALA O	-27.63	-23.65	81.46	15.00
105 ALA N	-25.55	-24.18	80.78	15.00
105 ALA CA	-25.91	-25.53	80.36	15.00
105 ALA CB	-26.98	-25.48	79.27	15.00
105 ALA C	-24.70	-26.30	79.86	15.00
105 ALA O	-23.56	-25.84	80.00	15.00
106 LYS N	-24.95	-27.48	79.33	15.00
106 LYS CA	-23.93	-28.36	78.78	15.00
106 LYS CB	-23.12	-29.05	79.90	15.00
106 LYS CG	-23.87	-30.12	80.70	15.00
106 LYS CD	-22.93	-30.93	81.56	15.00
106 LYS CE	-23.66	-31.74	82.65	15.00
106 LYS NZ	-24.38	-32.97	82.21	15.00
106 LYS C	-24.70	-29.41	77.99	15.00
106 LYS O	-25.89	-29.23	77.73	15.00
107 CYS N	-24.03	-30.47	77.57	15.00
107 CYS CA	-24.67	-31.55	76.85	15.00
107 CYS CB	-24.96	-31.18	75.39	15.00
107 CYS SG	-23.57	-31.18	74.26	15.00
107 CYS C	-23.77	-32.77	76.95	15.00
107 CYS O	-22.60	-32.67	77.31	15.00
108 ARG N	-24.35	-33.94	76.70	15.00
108 ARG CA	-23.62	-35.19	76.78	15.00
108 ARG CB	-24.30	-36.10	77.80	15.00
108 ARG CG	-24.56	-35.39	79.13	15.00

TABLE IV

108 ARG CD	-24.78	-36.37	80.25	15.00
108 ARG NE	-26.08	-37.03	80.17	15.00
108 ARG CZ	-26.31	-38.29	80.55	15.00
108 ARG NH1	-25.34	-39.05	81.03	15.00
108 ARG NH2	-27.55	-38.77	80.48	15.00
108 ARG C	-23.52	-35.88	75.42	15.00
108 ARG O	-23.75	-37.08	75.29	15.00
109 GLY N	-23.15	-35.11	74.40	15.00
109 GLY CA	-23.01	-35.66	73.07	15.00
109 GLY C	-23.96	-35.04	72.06	15.00
109 GLY O	-24.53	-33.97	72.30	15.00
110 TYR N	-24.12	-35.71	70.92	15.00
110 TYR CA	-24.99	-35.26	69.85	15.00
110 TYR CB	-24.28	-34.21	68.99	15.00
110 TYR CG	-23.06	-34.73	68.24	15.00
110 TYR CD1	-21.77	-34.40	68.67	15.00
110 TYR CE1	-20.65	-34.80	67.94	15.00
110 TYR CD2	-23.19	-35.48	67.08	15.00
110 TYR CE2	-22.08	-35.89	66.35	15.00
110 TYR CZ	-20.81	-35.54	66.79	15.00
110 TYR OH	-19.71	-35.91	66.03	15.00
110 TYR C	-25.41	-36.44	68.98	15.00
110 TYR O	-24.81	-37.52	69.04	15.00
111 ARG N	-26.39	-36.20	68.12	15.00
111 ARG CA	-26.91	-37.23	67.23	15.00
111 ARG CB	-28.22	-37.78	67.83	15.00
111 ARG CG	-28.86	-38.97	67.11	15.00
111 ARG CD	-29.48	-38.54	65.78	15.00
111 ARG NE	-30.34	-39.56	65.17	15.00
111 ARG CZ	-31.14	-39.34	64.13	15.00
111 ARG NH1	-31.19	-38.13	63.58	15.00
111 ARG NH2	-31.92	-40.30	63.68	15.00
111 ARG C	-27.13	-36.60	65.85	15.00
111 ARG O	-27.70	-35.51	65.74	15.00
112 GLU N	-26.67	-37.29	64.81	15.00
112 GLU CA	-26.82	-36.82	63.43	15.00
112 GLU CB	-25.52	-37.09	62.65	15.00
112 GLU CG	-24.30	-36.39	63.23	15.00
112 GLU CD	-23.02	-36.62	62.42	15.00
112 GLU OE1	-22.60	-35.70	61.69	15.00
112 GLU OE2	-22.42	-37.70	62.55	15.00
112 GLU C	-27.99	-37.52	62.76	15.00
112 GLU O	-28.31	-38.67	63.08	15.00

TABLE IV

113	ILE N	-28.66	-36.80	61.85	15.00
113	ILE CA	-29.79	-37.35	61.11	15.00
113	ILE CB	-30.77	-36.21	60.69	15.00
113	ILE CG2	-31.67	-36.67	59.56	15.00
113	ILE CG1	-31.62	-35.77	61.89	15.00
113	ILE CD1	-30.84	-35.23	63.06	15.00
113	ILE C	-29.26	-38.07	59.87	15.00
113	ILE O	-28.26	-37.65	59.27	15.00
114	PRO N	-29.88	-39.21	59.49	15.00
114	PRO CD	-31.02	-39.93	60.09	15.00
114	PRO CA	-29.39	-39.90	58.30	15.00
114	PRO CB	-30.43	-41.00	58.08	15.00
114	PRO CG	-30.91	-41.30	59.46	15.00
114	PRO C	-29.36	-38.89	57.15	15.00
114	PRO O	-30.36	-38.22	56.87	15.00
115	GLU N	-28.18	-38.70	56.57	15.00
115	GLU CA	-27.97	-37.75	55.49	15.00
115	GLU CB	-26.55	-37.89	54.96	15.00
115	GLU CG	-26.25	-37.14	53.69	15.00
115	GLU CD	-24.98	-37.66	53.04	15.00
115	GLU OE1	-25.08	-38.38	52.01	15.00
115	GLU OE2	-23.89	-37.37	53.58	15.00
115	GLU C	-28.99	-37.89	54.35	15.00
115	GLU O	-29.14	-38.97	53.79	15.00
116	GLY N	-29.66	-36.78	54.03	15.00
116	GLY CA	-30.66	-36.76	52.98	15.00
116	GLY C	-32.05	-37.27	53.37	15.00
116	GLY O	-33.00	-37.16	52.59	15.00
117	ASN N	-32.17	-37.77	54.60	15.00
117	ASN CA	-33.43	-38.32	55.09	15.00
117	ASN CB	-33.14	-39.42	56.11	15.00
117	ASN CG	-34.25	-40.47	56.18	15.00
117	ASN OD1	-35.40	-40.19	55.83	15.00
117	ASN ND2	-33.91	-41.67	56.64	15.00
117	ASN C	-34.36	-37.28	55.72	15.00
117	ASN O	-34.34	-37.10	56.93	15.00
118	GLU N	-35.19	-36.64	54.89	15.00
118	GLU CA	-36.16	-35.64	55.36	15.00
118	GLU CB	-36.86	-34.94	54.19	15.00
118	GLU CG	-36.01	-33.88	53.50	15.00
118	GLU CD	-36.83	-32.98	52.60	15.00
118	GLU OE1	-36.94	-33.27	51.39	15.00
118	GLU OE2	-37.37	-31.97	53.11	15.00

TABLE IV

118	GLU C	-37.21	-36.24	56.30	15.00
118	GLU O	-37.72	-35.57	57.19	15.00
119	LYS N	-37.53	-37.52	56.08	15.00
119	LYS CA	-38.47	-38.23	56.93	15.00
119	LYS CB	-38.64	-39.66	56.41	15.00
119	LYS CG	-39.73	-39.83	55.38	15.00
119	LYS CD	-39.53	-41.10	54.58	15.00
119	LYS CE	-38.51	-40.88	53.46	15.00
119	LYS NZ	-38.97	-39.83	52.48	15.00
119	LYS C	-37.91	-38.29	58.36	15.00
119	LYS O	-38.58	-37.89	59.32	15.00
120	ALA N	-36.70	-38.81	58.51	15.00
120	ALA CA	-36.06	-38.92	59.81	15.00
120	ALA CB	-34.71	-39.60	59.68	15.00
120	ALA C	-35.91	-37.54	60.41	15.00
120	ALA O	-36.06	-37.38	61.61	15.00
121	LEU N	-35.63	-36.55	59.56	15.00
121	LEU CA	-35.48	-35.17	60.05	15.00
121	LEU CB	-35.11	-34.21	58.90	15.00
121	LEU CG	-34.87	-32.75	59.33	15.00
121	LEU CD1	-33.74	-32.69	60.38	15.00
121	LEU CD2	-34.53	-31.88	58.12	15.00
121	LEU C	-36.78	-34.71	60.72	15.00
121	LEU O	-36.75	-34.17	61.83	15.00
122	LYS N	-37.91	-34.94	60.05	15.00
122	LYS CA	-39.23	-34.59	60.56	15.00
122	LYS CB	-40.31	-35.02	59.58	15.00
122	LYS CG	-41.74	-34.91	60.12	15.00
122	LYS CD	-42.72	-35.57	59.17	15.00
122	LYS CE	-44.11	-35.67	59.76	15.00
122	LYS NZ	-45.10	-36.14	58.74	15.00
122	LYS C	-39.44	-35.32	61.88	15.00
122	LYS O	-39.88	-34.74	62.87	15.00
123	ARG N	-39.14	-36.61	61.86	15.00
123	ARG CA	-39.28	-37.46	63.03	15.00
123	ARG CB	-38.80	-38.87	62.70	15.00
123	ARG CG	-38.84	-39.87	63.86	15.00
123	ARG CD	-37.70	-40.88	63.77	15.00
123	ARG NE	-37.37	-41.20	62.38	15.00
123	ARG CZ	-36.78	-42.32	61.98	15.00
123	ARG NH1	-36.45	-43.25	62.87	15.00
123	ARG NH2	-36.53	-42.51	60.69	15.00
123	ARG C	-38.46	-36.88	64.19	15.00

TABLE IV

123 ARG O	-38.93	-36.84	65.32	15.00
124 ALA N	-37.25	-36.42	63.89	15.00
124 ALA CA	-36.37	-35.84	64.90	15.00
124 ALA CB	-34.98	-35.61	64.35	15.00
124 ALA C	-36.95	-34.53	65.45	15.00
124 ALA O	-37.02	-34.33	66.66	15.00
125 VAL N	-37.41	-33.66	64.57	15.00
125 VAL CA	-37.99	-32.41	65.03	15.00
125 VAL CB	-38.35	-31.48	63.87	15.00
125 VAL CG1	-38.98	-30.19	64.39	15.00
125 VAL CG2	-37.09	-31.17	63.06	15.00
125 VAL C	-39.23	-32.65	65.89	15.00
125 VAL O	-39.46	-31.94	66.87	15.00
126 ALA N	-40.01	-33.67	65.53	15.00
126 ALA CA	-41.22	-34.03	66.25	15.00
126 ALA CB	-42.03	-35.02	65.44	15.00
126 ALA C	-40.89	-34.61	67.62	15.00
126 ALA O	-41.40	-34.14	68.64	15.00
127 ARG N	-40.03	-35.62	67.64	15.00
127 ARG CA	-39.61	-36.29	68.86	15.00
127 ARG CB	-38.83	-37.54	68.48	15.00
127 ARG CG	-38.45	-38.44	69.64	15.00
127 ARG CD	-39.63	-39.28	70.13	15.00
127 ARG NE	-40.15	-40.18	69.10	15.00
127 ARG CZ	-41.18	-39.90	68.31	15.00
127 ARG NH1	-41.59	-40.78	67.41	15.00
127 ARG NH2	-41.81	-38.73	68.42	15.00
127 ARG C	-38.75	-35.47	69.83	15.00
127 ARG O	-39.05	-35.36	71.01	15.00
128 VAL N	-37.64	-34.94	69.31	15.00
128 VAL CA	-36.66	-34.21	70.11	15.00
128 VAL CB	-35.23	-34.54	69.59	15.00
128 VAL CG1	-34.17	-33.72	70.32	15.00
128 VAL CG2	-34.95	-36.02	69.74	15.00
128 VAL C	-36.82	-32.70	70.26	15.00
128 VAL O	-36.73	-32.17	71.36	15.00
129 GLY N	-37.00	-32.01	69.14	15.00
129 GLY CA	-37.16	-30.56	69.20	15.00
129 GLY C	-36.36	-29.91	68.08	15.00
129 GLY O	-35.89	-30.62	67.18	15.00
130 PRO N	-36.19	-28.57	68.11	15.00
130 PRO CD	-36.66	-27.66	69.17	15.00
130 PRO CA	-35.45	-27.83	67.09	15.00

TABLE IV

130	PRO	CB	-35.23	-26.47	67.74	15.00
130	PRO	CG	-36.51	-26.30	68.52	15.00
130	PRO	C	-34.13	-28.52	66.74	15.00
130	PRO	O	-33.37	-28.91	67.63	15.00
131	VAL	N	-33.90	-28.72	65.45	15.00
131	VAL	CA	-32.71	-29.40	64.97	15.00
131	VAL	CB	-33.13	-30.65	64.15	15.00
131	VAL	CG1	-31.93	-31.36	63.57	15.00
131	VAL	CG2	-33.92	-31.61	65.03	15.00
131	VAL	C	-31.82	-28.49	64.13	15.00
131	VAL	O	-32.32	-27.69	63.34	15.00
132	SER	N	-30.51	-28.59	64.32	15.00
132	SER	CA	-29.56	-27.79	63.55	15.00
132	SER	CB	-28.18	-27.83	64.22	15.00
132	SER	OG	-28.20	-27.34	65.55	15.00
132	SER	C	-29.44	-28.37	62.14	15.00
132	SER	O	-29.41	-29.59	61.96	15.00
133	VAL	N	-29.39	-27.50	61.13	15.00
133	VAL	CA	-29.25	-27.94	59.75	15.00
133	VAL	CB	-30.63	-28.07	59.03	15.00
133	VAL	CG1	-31.40	-29.29	59.53	15.00
133	VAL	CG2	-31.45	-26.80	59.20	15.00
133	VAL	C	-28.37	-27.00	58.94	15.00
133	VAL	O	-28.12	-25.87	59.34	15.00
134	ALA	N	-27.86	-27.50	57.82	15.00
134	ALA	CA	-27.03	-26.73	56.91	15.00
134	ALA	CB	-25.65	-27.34	56.76	15.00
134	ALA	C	-27.75	-26.73	55.57	15.00
134	ALA	O	-28.29	-27.76	55.14	15.00
135	ILE	N	-27.80	-25.58	54.94	15.00
135	ILE	CA	-28.49	-25.45	53.66	15.00
135	ILE	CB	-29.82	-24.68	53.82	15.00
135	ILE	CG2	-30.80	-25.45	54.70	15.00
135	ILE	CG1	-29.52	-23.28	54.38	15.00
135	ILE	CD1	-30.72	-22.40	54.52	15.00
135	ILE	C	-27.64	-24.61	52.73	15.00
135	ILE	O	-26.59	-24.09	53.13	15.00
136	ASP	N	-28.09	-24.49	51.49	15.00
136	ASP	CA	-27.42	-23.66	50.51	15.00
136	ASP	CB	-27.50	-24.28	49.11	15.00
136	ASP	CG	-27.02	-23.32	48.02	15.00
136	ASP	OD1	-27.46	-23.49	46.88	15.00
136	ASP	OD2	-26.22	-22.40	48.29	15.00

TABLE IV

136 ASP C	-28.19	-22.36	50.54	15.00
136 ASP O	-29.34	-22.29	50.10	15.00
137 ALA N	-27.58	-21.33	51.11	15.00
137 ALA CA	-28.19	-20.02	51.21	15.00
137 ALA CB	-28.14	-19.54	52.65	15.00
137 ALA C	-27.47	-19.04	50.30	15.00
137 ALA O	-27.42	-17.85	50.60	15.00
138 SER N	-26.94	-19.53	49.20	15.00
138 SER CA	-26.20	-18.66	48.30	15.00
138 SER CB	-25.12	-19.44	47.57	15.00
138 SER OG	-25.71	-20.45	46.78	15.00
138 SER C	-27.06	-17.91	47.29	15.00
138 SER O	-26.76	-16.77	46.94	15.00
139 LEU N	-28.12	-18.55	46.82	15.00
139 LEU CA	-28.99	-17.95	45.82	15.00
139 LEU CB	-30.12	-18.91	45.46	15.00
139 LEU CG	-29.76	-20.02	44.48	15.00
139 LEU CD1	-29.30	-19.40	43.18	15.00
139 LEU CD2	-28.67	-20.89	45.03	15.00
139 LEU C	-29.56	-16.58	46.18	15.00
139 LEU O	-29.93	-16.32	47.33	15.00
140 THR N	-29.63	-15.71	45.19	15.00
140 THR CA	-30.19	-14.37	45.38	15.00
140 THR CB	-30.06	-13.54	44.09	15.00
140 THR OG1	-28.67	-13.30	43.82	15.00
140 THR CG2	-30.80	-12.20	44.20	15.00
140 THR C	-31.65	-14.43	45.86	15.00
140 THR O	-32.09	-13.62	46.69	15.00
141 SER N	-32.38	-15.45	45.40	15.00
141 SER CA	-33.77	-15.63	45.79	15.00
141 SER CB	-34.39	-16.77	44.99	15.00
141 SER OG	-33.78	-18.00	45.32	15.00
141 SER C	-33.89	-15.89	47.29	15.00
141 SER O	-34.94	-15.63	47.90	15.00
142 PHE N	-32.82	-16.43	47.89	15.00
142 PHE CA	-32.79	-16.70	49.33	15.00
142 PHE CB	-31.71	-17.72	49.67	15.00
142 PHE CG	-31.77	-18.20	51.08	15.00
142 PHE CD1	-32.45	-19.38	51.39	15.00
142 PHE CD2	-31.14	-17.49	52.10	15.00
142 PHE CE1	-32.51	-19.85	52.70	15.00
142 PHE CE2	-31.20	-17.95	53.41	15.00
142 PHE CZ	-31.88	-19.14	53.72	15.00

TABLE IV

142	PHE C	-32.53	-15.40	50.08	15.00
142	PHE O	-33.22	-15.09	51.06	15.00
143	GLN N	-31.55	-14.64	49.60	15.00
143	GLN CA	-31.19	-13.38	50.22	15.00
143	GLN CB	-30.07	-12.72	49.44	15.00
143	GLN CG	-29.68	-11.32	49.94	15.00
143	GLN CD	-28.36	-10.81	49.37	15.00
143	GLN OE1	-28.05	-9.62	49.47	15.00
143	GLN NE2	-27.56	-11.71	48.80	15.00
143	GLN C	-32.38	-12.43	50.33	15.00
143	GLN O	-32.57	-11.75	51.35	15.00
144	PHE N	-33.22	-12.40	49.30	15.00
144	PHE CA	-34.36	-11.50	49.31	15.00
144	PHE CB	-34.41	-10.73	47.98	15.00
144	PHE CG	-33.22	-9.85	47.75	15.00
144	PHE CD1	-33.13	-8.59	48.35	15.00
144	PHE CD2	-32.17	-10.27	46.94	15.00
144	PHE CE1	-32.02	-7.77	48.15	15.00
144	PHE CE2	-31.05	-9.46	46.73	15.00
144	PHE CZ	-30.98	-8.21	47.34	15.00
144	PHE C	-35.73	-12.13	49.64	15.00
144	PHE O	-36.77	-11.52	49.38	15.00
145	TYR N	-35.72	-13.30	50.26	15.00
145	TYR CA	-36.97	-13.98	50.63	15.00
145	TYR CB	-36.68	-15.35	51.26	15.00
145	TYR CG	-37.89	-15.98	51.94	15.00
145	TYR CD1	-38.72	-16.89	51.26	15.00
145	TYR CE1	-39.83	-17.45	51.89	15.00
145	TYR CD2	-38.21	-15.66	53.26	15.00
145	TYR CE2	-39.33	-16.22	53.90	15.00
145	TYR CZ	-40.13	-17.12	53.21	15.00
145	TYR OH	-41.21	-17.68	53.85	15.00
145	TYR C	-37.81	-13.16	51.62	15.00
145	TYR O	-37.27	-12.49	52.50	15.00
146	SER N	-39.13	-13.26	51.50	15.00
146	SER CA	-40.03	-12.55	52.41	15.00
146	SER CB	-40.33	-11.12	51.96	15.00
146	SER OG	-40.50	-11.03	50.57	15.00
146	SER C	-41.31	-13.30	52.73	15.00
146	SER O	-41.74	-13.31	53.88	15.00
147	LYS N	-41.89	-14.00	51.76	15.00
147	LYS CA	-43.13	-14.74	51.99	15.00
147	LYS CB	-44.34	-13.80	51.82	15.00

TABLE IV

147	LYS	CG	-44.60	-12.90	53.05	15.00
147	LYS	CD	-45.56	-11.75	52.75	15.00
147	LYS	CE	-45.63	-10.76	53.91	15.00
147	LYS	NZ	-46.25	-11.32	55.15	15.00
147	LYS	C	-43.30	-15.99	51.13	15.00
147	LYS	O	-42.68	-16.13	50.07	15.00
148	GLY	N	-44.12	-16.92	51.60	15.00
148	GLY	CA	-44.36	-18.14	50.87	15.00
148	GLY	C	-43.35	-19.22	51.18	15.00
148	GLY	O	-42.39	-19.00	51.90	15.00
149	VAL	N	-43.60	-20.42	50.67	15.00
149	VAL	CA	-42.69	-21.53	50.90	15.00
149	VAL	CB	-43.43	-22.89	50.72	15.00
149	VAL	CG1	-42.46	-24.05	50.79	15.00
149	VAL	CG2	-44.49	-23.05	51.80	15.00
149	VAL	C	-41.56	-21.34	49.88	15.00
149	VAL	O	-41.81	-21.30	48.67	15.00
150	TYR	N	-40.34	-21.13	50.37	15.00
150	TYR	CA	-39.19	-20.92	49.50	15.00
150	TYR	CB	-37.99	-20.42	50.30	15.00
150	TYR	CG	-36.72	-20.27	49.46	15.00
150	TYR	CD1	-36.48	-19.11	48.72	15.00
150	TYR	CE1	-35.31	-18.98	47.96	15.00
150	TYR	CD2	-35.77	-21.30	49.41	15.00
150	TYR	CE2	-34.59	-21.17	48.65	15.00
150	TYR	CZ	-34.37	-20.01	47.93	15.00
150	TYR	OH	-33.22	-19.88	47.19	15.00
150	TYR	C	-38.80	-22.18	48.76	15.00
150	TYR	O	-38.87	-23.29	49.30	15.00
151	TYR	N	-38.31	-21.98	47.54	15.00
151	TYR	CA	-37.87	-23.07	46.68	15.00
151	TYR	CB	-39.07	-23.95	46.31	15.00
151	TYR	CG	-38.80	-25.01	45.27	15.00
151	TYR	CD1	-38.36	-26.28	45.62	15.00
151	TYR	CE1	-38.19	-27.27	44.66	15.00
151	TYR	CD2	-39.05	-24.75	43.92	15.00
151	TYR	CE2	-38.88	-25.73	42.96	15.00
151	TYR	CZ	-38.46	-26.98	43.33	15.00
151	TYR	OH	-38.34	-27.95	42.36	15.00
151	TYR	C	-37.24	-22.44	45.44	15.00
151	TYR	O	-37.66	-21.37	45.00	15.00
152	ASP	N	-36.22	-23.11	44.89	15.00
152	ASP	CA	-35.52	-22.62	43.70	15.00

TABLE IV

152 ASP CB	-34.55	-21.50	44.08	15.00
152 ASP CG	-33.97	-20.77	42.87	15.00
152 ASP OD1	-33.75	-21.39	41.81	15.00
152 ASP OD2	-33.72	-19.56	42.99	15.00
152 ASP C	-34.75	-23.77	43.07	15.00
152 ASP O	-33.90	-24.38	43.73	15.00
153 GLU N	-35.01	-24.02	41.79	15.00
153 GLU CA	-34.35	-25.09	41.04	15.00
153 GLU CB	-34.78	-25.06	39.56	15.00
153 GLU CG	-36.22	-25.45	39.26	15.00
153 GLU CD	-36.59	-25.21	37.78	15.00
153 GLU OE1	-37.05	-24.09	37.45	15.00
153 GLU OE2	-36.40	-26.14	36.96	15.00
153 GLU C	-32.84	-24.95	41.09	15.00
153 GLU O	-32.12	-25.93	40.99	15.00
154 SER N	-32.38	-23.71	41.20	15.00
154 SER CA	-30.95	-23.41	41.24	15.00
154 SER CB	-30.73	-21.93	40.92	15.00
154 SER OG	-31.33	-21.57	39.69	15.00
154 SER C	-30.25	-23.78	42.55	15.00
154 SER O	-29.02	-23.75	42.63	15.00
155 CYS N	-31.02	-24.11	43.58	15.00
155 CYS CA	-30.44	-24.46	44.87	15.00
155 CYS C	-29.58	-25.72	44.76	15.00
155 CYS O	-29.98	-26.72	44.17	15.00
155 CYS CB	-31.53	-24.65	45.92	15.00
155 CYS SG	-31.12	-23.81	47.48	15.00
156 ASN N	-28.40	-25.67	45.35	15.00
156 ASN CA	-27.48	-26.80	45.29	15.00
156 ASN CB	-26.09	-26.28	44.91	15.00
156 ASN CG	-25.15	-27.39	44.45	15.00
156 ASN OD1	-25.21	-28.54	44.94	15.00
156 ASN ND2	-24.26	-27.05	43.53	15.00
156 ASN C	-27.42	-27.58	46.61	15.00
156 ASN O	-26.99	-27.06	47.64	15.00
157 SER N	-27.80	-28.85	46.54	15.00
157 SER CA	-27.82	-29.72	47.71	15.00
157 SER CB	-28.66	-30.98	47.45	15.00
157 SER OG	-28.07	-31.81	46.47	15.00
157 SER C	-26.43	-30.14	48.17	15.00
157 SER O	-26.27	-30.76	49.23	15.00
158 ASP N	-25.42	-29.82	47.37	15.00
158 ASP CA	-24.06	-30.18	47.69	15.00

TABLE IV

158 ASP CB	-23.44	-30.99	46.55	15.00
158 ASP CG	-23.70	-32.49	46.69	15.00
158 ASP OD1	-24.30	-33.11	45.78	15.00
158 ASP OD2	-23.32	-33.05	47.75	15.00
158 ASP C	-23.21	-29.01	48.14	15.00
158 ASP O	-22.19	-29.21	48.79	15.00
159 ASN N	-23.67	-27.80	47.85	15.00
159 ASN CA	-22.95	-26.60	48.28	15.00
159 ASN CB	-23.04	-25.49	47.22	15.00
159 ASN CG	-22.27	-24.23	47.61	15.00
159 ASN OD1	-21.81	-24.09	48.74	15.00
159 ASN ND2	-22.14	-23.31	46.67	15.00
159 ASN C	-23.55	-26.10	49.61	15.00
159 ASN O	-24.20	-25.06	49.67	15.00
160 LEU N	-23.38	-26.89	50.68	15.00
160 LEU CA	-23.91	-26.47	51.98	15.00
160 LEU CB	-23.83	-27.61	52.99	15.00
160 LEU CG	-24.49	-28.94	52.62	15.00
160 LEU CD1	-24.41	-29.89	53.81	15.00
160 LEU CD2	-25.94	-28.71	52.23	15.00
160 LEU C	-23.04	-25.30	52.41	15.00
160 LEU O	-21.82	-25.42	52.46	15.00
161 ASN N	-23.65	-24.15	52.70	15.00
161 ASN CA	-22.86	-22.98	53.07	15.00
161 ASN CB	-22.59	-22.13	51.83	15.00
161 ASN CG	-23.82	-21.92	50.98	15.00
161 ASN OD1	-24.77	-21.24	51.38	15.00
161 ASN ND2	-23.83	-22.51	49.81	15.00
161 ASN C	-23.40	-22.10	54.20	15.00
161 ASN O	-22.80	-21.07	54.54	15.00
162 HIS N	-24.47	-22.55	54.85	15.00
162 HIS CA	-25.07	-21.78	55.92	15.00
162 HIS CB	-26.12	-20.83	55.33	15.00
162 HIS CG	-26.58	-19.75	56.27	15.00
162 HIS CD2	-27.81	-19.22	56.48	15.00
162 HIS ND1	-25.73	-19.08	57.12	15.00
162 HIS CE1	-26.41	-18.20	57.83	15.00
162 HIS NE2	-27.68	-18.27	57.46	15.00
162 HIS C	-25.71	-22.76	56.91	15.00
162 HIS O	-26.37	-23.71	56.50	15.00
163 ALA N	-25.40	-22.58	58.19	15.00
163 ALA CA	-25.96	-23.43	59.24	15.00
163 ALA CB	-24.95	-23.66	60.35	15.00

TABLE IV

163 ALA C	-27.17	-22.65	59.74	15.00
163 ALA O	-27.10	-21.42	59.92	15.00
164 VAL N	-28.27	-23.34	59.96	15.00
164 VAL CA	-29.51	-22.71	60.36	15.00
164 VAL CB	-30.30	-22.38	59.08	15.00
164 VAL CG1	-31.28	-23.48	58.75	15.00
164 VAL CG2	-30.90	-20.99	59.15	15.00
164 VAL C	-30.30	-23.60	61.34	15.00
164 VAL O	-29.89	-24.73	61.62	15.00
165 LEU N	-31.40	-23.09	61.89	15.00
165 LEU CA	-32.18	-23.86	62.86	15.00
165 LEU CB	-32.27	-23.11	64.20	15.00
165 LEU CG	-32.79	-23.87	65.44	15.00
165 LEU CD1	-31.76	-24.89	65.90	15.00
165 LEU CD2	-33.13	-22.90	66.57	15.00
165 LEU C	-33.58	-24.27	62.40	15.00
165 LEU O	-34.39	-23.42	62.03	15.00
166 ALA N	-33.85	-25.57	62.43	15.00
166 ALA CA	-35.15	-26.11	62.05	15.00
166 ALA CB	-35.00	-27.51	61.50	15.00
166 ALA C	-35.99	-26.11	63.33	15.00
166 ALA O	-35.76	-26.91	64.25	15.00
167 VAL N	-36.94	-25.19	63.39	15.00
167 VAL CA	-37.80	-25.06	64.55	15.00
167 VAL CB	-37.81	-23.60	65.03	15.00
167 VAL CG1	-38.83	-22.75	64.24	15.00
167 VAL CG2	-38.06	-23.55	66.50	15.00
167 VAL C	-39.23	-25.58	64.33	15.00
167 VAL O	-40.15	-25.31	65.14	15.00
168 GLY N	-39.44	-26.31	63.24	15.00
168 GLY CA	-40.76	-26.84	62.97	15.00
168 GLY C	-40.97	-27.25	61.53	15.00
168 GLY O	-40.02	-27.37	60.74	15.00
169 TYR N	-42.23	-27.48	61.20	15.00
169 TYR CA	-42.67	-27.89	59.87	15.00
169 TYR CB	-42.21	-29.33	59.54	15.00
169 TYR CG	-42.75	-30.41	60.46	15.00
169 TYR CD1	-43.94	-31.09	60.16	15.00
169 TYR CE1	-44.43	-32.10	60.99	15.00
169 TYR CD2	-42.06	-30.79	61.61	15.00
169 TYR CE2	-42.53	-31.80	62.45	15.00
169 TYR CZ	-43.71	-32.45	62.13	15.00
169 TYR OH	-44.15	-33.47	62.94	15.00

TABLE IV

169 TYR C	-44.18	-27.80	59.84	15.00
169 TYR O	-44.84	-27.82	60.88	15.00
170 GLY N	-44.73	-27.73	58.64	15.00
170 GLY CA	-46.17	-27.63	58.48	15.00
170 GLY C	-46.53	-27.64	57.01	15.00
170 GLY O	-45.73	-28.04	56.18	15.00
171 ILE N	-47.71	-27.14	56.69	15.00
171 ILE CA	-48.16	-27.09	55.30	15.00
171 ILE CB	-48.95	-28.37	54.91	15.00
171 ILE CG2	-50.04	-28.69	55.91	15.00
171 ILE CG1	-49.52	-28.25	53.51	15.00
171 ILE CD1	-50.20	-29.53	53.05	15.00
171 ILE C	-48.97	-25.82	55.09	15.00
171 ILE O	-49.84	-25.48	55.89	15.00
172 GLN N	-48.59	-25.07	54.05	15.00
172 GLN CA	-49.21	-23.80	53.72	15.00
172 GLN CB	-48.19	-22.67	53.89	15.00
172 GLN CG	-48.68	-21.32	53.45	15.00
172 GLN CD	-47.73	-20.20	53.84	15.00
172 GLN OE1	-47.84	-19.61	54.92	15.00
172 GLN NE2	-46.78	-19.89	52.96	15.00
172 GLN C	-49.73	-23.81	52.29	15.00
172 GLN O	-48.96	-23.96	51.33	15.00
173 LYS N	-51.04	-23.64	52.17	15.00
173 LYS CA	-51.73	-23.62	50.88	15.00
173 LYS CB	-51.37	-22.35	50.09	15.00
173 LYS CG	-51.48	-21.01	50.88	15.00
173 LYS CD	-52.85	-20.77	51.55	15.00
173 LYS CE	-54.02	-20.84	50.56	15.00
173 LYS NZ	-53.89	-19.90	49.41	15.00
173 LYS C	-51.39	-24.87	50.08	15.00
173 LYS O	-51.27	-24.82	48.87	15.00
174 GLY N	-51.22	-25.99	50.77	15.00
174 GLY CA	-50.91	-27.24	50.10	15.00
174 GLY C	-49.43	-27.58	50.06	15.00
174 GLY O	-49.07	-28.71	49.74	15.00
175 ASN N	-48.59	-26.65	50.48	15.00
175 ASN CA	-47.15	-26.87	50.44	15.00
175 ASN CB	-46.44	-25.64	49.88	15.00
175 ASN CG	-47.06	-25.14	48.59	15.00
175 ASN OD1	-47.08	-25.86	47.58	15.00
175 ASN ND2	-47.56	-23.91	48.62	15.00
175 ASN C	-46.54	-27.23	51.79	15.00

TABLE IV

175 ASN O	-46.63	-26.46	52.74	15.00
176 LYS N	-45.92	-28.40	51.87	15.00
176 LYS CA	-45.28	-28.84	53.09	15.00
176 LYS CB	-44.98	-30.33	53.02	15.00
176 LYS CG	-46.23	-31.18	52.84	15.00
176 LYS CD	-45.95	-32.63	53.09	15.00
176 LYS CE	-47.17	-33.48	52.82	15.00
176 LYS NZ	-46.84	-34.93	52.78	15.00
176 LYS C	-44.00	-28.03	53.20	15.00
176 LYS O	-43.37	-27.73	52.19	15.00
177 HIS N	-43.59	-27.69	54.42	15.00
177 HIS CA	-42.39	-26.88	54.58	15.00
177 HIS CB	-42.76	-25.39	54.51	15.00
177 HIS CG	-43.62	-24.94	55.64	15.00
177 HIS CD2	-43.32	-24.68	56.94	15.00
177 HIS ND1	-44.96	-24.70	55.50	15.00
177 HIS CE1	-45.46	-24.31	56.66	15.00
177 HIS NE2	-44.48	-24.29	57.55	15.00
177 HIS C	-41.68	-27.10	55.88	15.00
177 HIS O	-42.20	-27.76	56.78	15.00
178 TRP N	-40.52	-26.46	55.99	15.00
178 TRP CA	-39.69	-26.51	57.18	15.00
178 TRP CB	-38.24	-26.84	56.79	15.00
178 TRP CG	-38.01	-28.23	56.31	15.00
178 TRP CD2	-38.14	-29.45	57.06	15.00
178 TRP CE2	-37.73	-30.50	56.22	15.00
178 TRP CE3	-38.56	-29.74	58.37	15.00
178 TRP CD1	-37.55	-28.59	55.07	15.00
178 TRP NE1	-37.38	-29.95	55.01	15.00
178 TRP CZ2	-37.73	-31.85	56.64	15.00
178 TRP CZ3	-38.56	-31.08	58.79	15.00
178 TRP CH2	-38.14	-32.12	57.92	15.00
178 TRP C	-39.73	-25.11	57.74	15.00
178 TRP O	-39.68	-24.14	56.97	15.00
179 ILE N	-39.90	-24.97	59.05	15.00
179 ILE CA	-39.91	-23.65	59.65	15.00
179 ILE CB	-40.89	-23.55	60.84	15.00
179 ILE CG2	-40.95	-22.10	61.34	15.00
179 ILE CG1	-42.29	-24.02	60.43	15.00
179 ILE CD1	-43.32	-23.95	61.55	15.00
179 ILE C	-38.47	-23.41	60.08	15.00
179 ILE O	-37.96	-24.05	61.00	15.00
180 ILE N	-37.79	-22.52	59.36	15.00

TABLE IV

180 ILE CA	-36.40	-22.23	59.61	15.00
180 ILE CB	-35.58	-22.34	58.29	15.00
180 ILE CG2	-34.14	-21.97	58.52	15.00
180 ILE CG1	-35.74	-23.74	57.68	15.00
180 ILE CD1	-35.52	-24.88	58.66	15.00
180 ILE C	-36.13	-20.88	60.25	15.00
180 ILE O	-36.68	-19.85	59.84	15.00
181 LYS N	-35.24	-20.90	61.25	15.00
181 LYS CA	-34.84	-19.72	61.99	15.00
181 LYS CB	-34.77	-20.06	63.48	15.00
181 LYS CG	-34.66	-18.84	64.35	15.00
181 LYS CD	-34.34	-19.17	65.79	15.00
181 LYS CE	-34.16	-17.89	66.56	15.00
181 LYS NZ	-33.69	-18.09	67.94	15.00
181 LYS C	-33.46	-19.27	61.49	15.00
181 LYS O	-32.50	-20.03	61.56	15.00
182 ASN N	-33.37	-18.05	60.98	15.00
182 ASN CA	-32.11	-17.52	60.47	15.00
182 ASN CB	-32.33	-16.76	59.15	15.00
182 ASN CG	-31.05	-16.64	58.29	15.00
182 ASN OD1	-30.00	-17.21	58.60	15.00
182 ASN ND2	-31.15	-15.91	57.18	15.00
182 ASN C	-31.43	-16.62	61.51	15.00
182 ASN O	-32.00	-16.33	62.57	15.00
183 SER N	-30.18	-16.25	61.24	15.00
183 SER CA	-29.43	-15.38	62.14	15.00
183 SER CB	-28.25	-16.13	62.75	15.00
183 SER OG	-27.48	-16.78	61.76	15.00
183 SER C	-28.96	-14.09	61.44	15.00
183 SER O	-27.85	-13.63	61.66	15.00
184 TRP N	-29.82	-13.52	60.59	15.00
184 TRP CA	-29.50	-12.28	59.88	15.00
184 TRP CB	-29.69	-12.45	58.37	15.00
184 TRP CG	-28.71	-13.44	57.76	15.00
184 TRP CD2	-28.74	-13.98	56.44	15.00
184 TRP CE2	-27.62	-14.83	56.30	15.00
184 TRP CE3	-29.60	-13.83	55.34	15.00
184 TRP CD1	-27.60	-13.98	58.37	15.00
184 TRP NE1	-26.95	-14.81	57.50	15.00
184 TRP CZ2	-27.34	-15.53	55.13	15.00
184 TRP CZ3	-29.33	-14.52	54.17	15.00
184 TRP CH2	-28.21	-15.35	54.07	15.00
184 TRP C	-30.35	-11.11	60.40	15.00

TABLE IV

184 TRP O	-30.51	-10.09	59.72	15.00
185 GLY N	-30.84	-11.25	61.63	15.00
185 GLY CA	-31.67	-10.22	62.24	15.00
185 GLY C	-33.14	-10.43	61.94	15.00
185 GLY O	-33.49	-11.18	61.03	15.00
186 GLU N	-33.99	-9.73	62.68	15.00
186 GLU CA	-35.45	-9.83	62.50	15.00
186 GLU CB	-36.17	-9.31	63.74	15.00
186 GLU CG	-35.94	-10.14	64.97	15.00
186 GLU CD	-37.15	-10.15	65.89	15.00
186 GLU OE1	-38.26	-10.52	65.41	15.00
186 GLU OE2	-37.01	-9.81	67.09	15.00
186 GLU C	-36.05	-9.15	61.27	15.00
186 GLU O	-37.10	-9.56	60.78	15.00
187 ASN N	-35.38	-8.12	60.76	15.00
187 ASN CA	-35.89	-7.42	59.59	15.00
187 ASN CB	-35.32	-6.00	59.52	15.00
187 ASN CG	-35.95	-5.04	60.53	15.00
187 ASN OD1	-35.82	-3.83	60.39	15.00
187 ASN ND2	-36.62	-5.58	61.56	15.00
187 ASN C	-35.60	-8.14	58.29	15.00
187 ASN O	-35.82	-7.57	57.22	15.00
188 TRP N	-35.12	-9.38	58.37	15.00
188 TRP CA	-34.81	-10.18	57.17	15.00
188 TRP CB	-33.42	-10.84	57.28	15.00
188 TRP CG	-33.16	-11.85	56.18	15.00
188 TRP CD2	-33.54	-13.23	56.17	15.00
188 TRP CE2	-33.19	-13.75	54.89	15.00
188 TRP CE3	-34.14	-14.09	57.10	15.00
188 TRP CD1	-32.60	-11.59	54.97	15.00
188 TRP NE1	-32.63	-12.73	54.18	15.00
188 TRP CZ2	-33.44	-15.08	54.52	15.00
188 TRP CZ3	-34.39	-15.42	56.74	15.00
188 TRP CH2	-34.03	-15.90	55.46	15.00
188 TRP C	-35.88	-11.27	57.03	15.00
188 TRP O	-36.45	-11.71	58.04	15.00
189 GLY N	-36.14	-11.69	55.79	15.00
189 GLY CA	-37.13	-12.72	55.53	15.00
189 GLY C	-38.45	-12.40	56.21	15.00
189 GLY O	-38.91	-11.26	56.15	15.00
190 ASN N	-39.07	-13.38	56.85	15.00
190 ASN CA	-40.33	-13.14	57.55	15.00
190 ASN CB	-41.33	-14.27	57.29	15.00

TABLE IV

190 ASN CG	-42.74	-13.89	57.69	15.00
190 ASN OD1	-42.98	-12.88	58.35	15.00
190 ASN ND2	-43.69	-14.70	57.26	15.00
190 ASN C	-40.03	-13.04	59.04	15.00
190 ASN O	-40.09	-14.04	59.76	15.00
191 LYS N	-39.68	-11.83	59.49	15.00
191 LYS CA	-39.34	-11.59	60.90	15.00
191 LYS CB	-40.57	-11.79	61.81	15.00
191 LYS CG	-41.66	-10.76	61.63	15.00
191 LYS CD	-42.98	-11.23	62.27	15.00
191 LYS CE	-43.69	-12.29	61.41	15.00
191 LYS NZ	-42.88	-13.54	61.16	15.00
191 LYS C	-38.18	-12.50	61.33	15.00
191 LYS O	-38.18	-13.07	62.44	15.00
192 GLY N	-37.22	-12.67	60.43	15.00
192 GLY CA	-36.06	-13.51	60.71	15.00
192 GLY C	-36.27	-14.99	60.45	15.00
192 GLY O	-35.41	-15.81	60.78	15.00
193 TYR N	-37.40	-15.34	59.87	15.00
193 TYR CA	-37.69	-16.74	59.58	15.00
193 TYR CB	-38.93	-17.20	60.33	15.00
193 TYR CG	-38.68	-17.49	61.78	15.00
193 TYR CD1	-38.81	-16.48	62.74	15.00
193 TYR CE1	-38.56	-16.73	64.09	15.00
193 TYR CD2	-38.31	-18.77	62.20	15.00
193 TYR CE2	-38.06	-19.03	63.55	15.00
193 TYR CZ	-38.18	-18.01	64.48	15.00
193 TYR OH	-37.91	-18.26	65.81	15.00
193 TYR C	-37.92	-16.95	58.10	15.00
193 TYR O	-38.22	-16.01	57.36	15.00
194 ILE N	-37.81	-18.21	57.68	15.00
194 ILE CA	-38.04	-18.60	56.31	15.00
194 ILE CB	-36.73	-18.55	55.43	15.00
194 ILE CG2	-35.60	-19.33	56.09	15.00
194 ILE CG1	-37.01	-19.10	54.03	15.00
194 ILE CD1	-35.85	-18.96	53.07	15.00
194 ILE C	-38.63	-20.00	56.30	15.00
194 ILE O	-38.16	-20.88	57.01	15.00
195 LEU N	-39.72	-20.18	55.55	15.00
195 LEU CA	-40.34	-21.49	55.42	15.00
195 LEU CB	-41.87	-21.37	55.28	15.00
195 LEU CG	-42.73	-20.47	56.17	15.00
195 LEU CD1	-44.18	-20.60	55.73	15.00

TABLE IV

195 LEU CD2	-42.58	-20.81	57.65	15.00
195 LEU C	-39.76	-22.05	54.13	15.00
195 LEU O	-39.93	-21.45	53.06	15.00
196 MET N	-39.03	-23.15	54.22	15.00
196 MET CA	-38.43	-23.75	53.02	15.00
196 MET CB	-36.94	-24.02	53.26	15.00
196 MET CG	-36.14	-22.77	53.55	15.00
196 MET SD	-34.44	-23.13	54.06	15.00
196 MET CE	-33.70	-23.51	52.45	15.00
196 MET C	-39.16	-25.05	52.64	15.00
196 MET O	-39.62	-25.77	53.52	15.00
197 ALA N	-39.26	-25.34	51.35	15.00
197 ALA CA	-39.95	-26.53	50.86	15.00
197 ALA CB	-39.82	-26.63	49.36	15.00
197 ALA C	-39.52	-27.84	51.52	15.00
197 ALA O	-38.32	-28.08	51.73	15.00
198 ARG N	-40.50	-28.68	51.85	15.00
198 ARG CA	-40.27	-29.98	52.48	15.00
198 ARG CB	-41.04	-30.07	53.81	15.00
198 ARG CG	-41.06	-31.45	54.43	15.00
198 ARG CD	-41.33	-31.38	55.94	15.00
198 ARG NE	-42.61	-30.75	56.26	15.00
198 ARG CZ	-43.75	-31.42	56.44	15.00
198 ARG NH1	-43.78	-32.74	56.32	15.00
198 ARG NH2	-44.87	-30.76	56.70	15.00
198 ARG C	-40.73	-31.09	51.56	15.00
198 ARG O	-41.79	-31.00	50.96	15.00
199 ASN N	-39.95	-32.17	51.52	15.00
199 ASN CA	-40.22	-33.33	50.68	15.00
199 ASN CB	-41.58	-33.97	50.99	15.00
199 ASN CG	-41.67	-34.52	52.39	15.00
199 ASN OD1	-40.69	-34.50	53.14	15.00
199 ASN ND2	-42.85	-34.99	52.77	15.00
199 ASN C	-40.16	-32.94	49.21	15.00
199 ASN O	-40.84	-33.53	48.36	15.00
200 LYS N	-39.35	-31.93	48.91	15.00
200 LYS CA	-39.21	-31.49	47.55	15.00
200 LYS CB	-39.47	-29.99	47.43	15.00
200 LYS CG	-40.30	-29.64	46.22	15.00
200 LYS CD	-41.12	-28.37	46.46	15.00
200 LYS CE	-42.16	-28.18	45.36	15.00
200 LYS NZ	-41.56	-28.02	43.99	15.00
200 LYS C	-37.78	-31.85	47.17	15.00

TABLE IV

200 LYS O	-36.94	-30.98	46.93	15.00
201 ASN N	-37.51	-33.15	47.20	15.00
201 ASN CA	-36.21	-33.69	46.86	15.00
201 ASN CB	-35.94	-33.51	45.37	15.00
201 ASN CG	-36.89	-34.30	44.52	15.00
201 ASN OD1	-37.20	-35.46	44.81	15.00
201 ASN ND2	-37.40	-33.66	43.47	15.00
201 ASN C	-35.03	-33.16	47.67	15.00
201 ASN O	-33.94	-32.96	47.11	15.00
202 ASN N	-35.23	-33.00	48.98	15.00
202 ASN CA	-34.18	-32.51	49.89	15.00
202 ASN CB	-33.04	-33.54	49.99	15.00
202 ASN CG	-32.05	-33.23	51.10	15.00
202 ASN OD1	-32.41	-32.67	52.14	15.00
202 ASN ND2	-30.79	-33.59	50.89	15.00
202 ASN C	-33.66	-31.16	49.41	15.00
202 ASN O	-32.46	-30.95	49.27	15.00
203 ALA N	-34.57	-30.23	49.18	15.00
203 ALA H	-35.42	-30.45	49.60	15.00
203 ALA CA	-34.31	-28.90	48.63	15.00
203 ALA CB	-35.55	-28.01	48.72	15.00
203 ALA C	-33.20	-28.21	49.44	15.00
203 ALA O	-33.27	-28.01	50.64	15.00
204 CYS N	-32.19	-27.72	48.68	15.00
204 CYS CA	-31.05	-26.98	49.22	15.00
204 CYS C	-30.21	-27.75	50.22	15.00
204 CYS O	-29.44	-27.14	50.97	15.00
204 CYS CB	-31.51	-25.67	49.86	15.00
204 CYS SG	-32.47	-24.53	48.82	15.00
205 GLY N	-30.37	-29.07	50.27	15.00
205 GLY CA	-29.60	-29.89	51.20	15.00
205 GLY C	-30.01	-29.85	52.66	15.00
205 GLY O	-29.23	-30.21	53.55	15.00
206 ILE N	-31.27	-29.50	52.90	15.00
206 ILE CA	-31.84	-29.38	54.25	15.00
206 ILE CB	-33.38	-29.05	54.17	15.00
206 ILE CG2	-34.13	-30.21	53.53	15.00
206 ILE CG1	-33.94	-28.69	55.54	15.00
206 ILE CD1	-33.54	-27.31	56.02	15.00
206 ILE C	-31.59	-30.57	55.19	15.00
206 ILE O	-31.42	-30.39	56.40	15.00
207 ALA N	-31.52	-31.77	54.64	15.00
207 ALA CA	-31.27	-32.95	55.49	15.00

TABLE IV

207 ALA CB	-32.38	-33.99	55.31	15.00
207 ALA C	-29.89	-33.58	55.26	15.00
207 ALA O	-29.62	-34.70	55.70	15.00
208 ASN N	-28.99	-32.84	54.62	15.00
208 ASN CA	-27.66	-33.36	54.34	15.00
208 ASN CB	-27.05	-32.65	53.13	15.00
208 ASN CG	-27.49	-33.27	51.83	15.00
208 ASN OD1	-27.92	-34.43	51.79	15.00
208 ASN ND2	-27.39	-32.51	50.75	15.00
208 ASN C	-26.67	-33.32	55.51	15.00
208 ASN O	-25.80	-34.19	55.61	15.00
209 LEU N	-26.82	-32.35	56.40	15.00
209 LEU CA	-25.92	-32.20	57.53	15.00
209 LEU CB	-24.79	-31.22	57.16	15.00
209 LEU CG	-23.53	-31.18	58.02	15.00
209 LEU CD1	-22.72	-32.44	57.77	15.00
209 LEU CD2	-22.72	-29.93	57.68	15.00
209 LEU C	-26.69	-31.68	58.75	15.00
209 LEU O	-26.54	-30.52	59.15	15.00
210 ALA N	-27.50	-32.55	59.34	15.00
210 ALA H	-27.89	-32.98	58.56	15.00
210 ALA CA	-28.32	-32.12	60.48	15.00
210 ALA CB	-29.80	-32.37	60.21	15.00
210 ALA C	-27.94	-32.94	61.72	15.00
210 ALA O	-27.57	-34.09	61.63	15.00
211 SER N	-28.10	-32.29	62.88	15.00
211 SER CA	-27.80	-32.92	64.15	15.00
211 SER CB	-26.28	-32.97	64.37	15.00
211 SER OG	-25.71	-31.66	64.34	15.00
211 SER C	-28.46	-32.19	65.33	15.00
211 SER O	-29.01	-31.09	65.17	15.00
212 PHE N	-28.43	-32.83	66.50	15.00
212 PHE CA	-28.98	-32.24	67.71	15.00
212 PHE CB	-30.46	-32.59	67.86	15.00
212 PHE CG	-30.74	-34.06	67.93	15.00
212 PHE CD1	-31.03	-34.79	66.77	15.00
212 PHE CD2	-30.76	-34.72	69.16	15.00
212 PHE CE1	-31.34	-36.13	66.83	15.00
212 PHE CE2	-31.06	-36.08	69.22	15.00
212 PHE CZ	-31.35	-36.79	68.05	15.00
212 PHE C	-28.18	-32.66	68.96	15.00
212 PHE O	-27.65	-33.77	69.03	15.00
213 PRO N	-28.03	-31.76	69.92	15.00

TABLE IV

213	PRO	CD	-28.51	-30.37	69.98	15.00
213	PRO	CA	-27.28	-32.11	71.13	15.00
213	PRO	CB	-27.07	-30.76	71.79	15.00
213	PRO	CG	-28.33	-30.03	71.43	15.00
213	PRO	C	-28.10	-33.03	72.01	15.00
213	PRO	O	-29.33	-33.00	71.95	15.00
214	LYS	N	-27.42	-33.86	72.80	15.00
214	LYS	CA	-28.08	-34.78	73.73	15.00
214	LYS	CB	-27.64	-36.23	73.50	15.00
214	LYS	CG	-27.92	-36.75	72.10	15.00
214	LYS	CD	-27.72	-38.26	72.00	15.00
214	LYS	CE	-26.29	-38.66	72.30	15.00
214	LYS	NZ	-26.00	-39.99	71.69	15.00
214	LYS	C	-27.60	-34.34	75.10	15.00
214	LYS	O	-26.43	-34.00	75.26	15.00
215	MET	N	-28.50	-34.30	76.07	15.00
215	MET	CA	-28.12	-33.90	77.42	15.00
215	MET	CB	-28.97	-32.72	77.89	15.00
215	MET	CG	-28.96	-31.51	76.95	15.00
215	MET	SD	-29.63	-30.02	77.75	15.00
215	MET	CE	-28.68	-28.69	76.95	15.00
215	MET	C	-28.26	-35.09	78.36	15.00
215	MET	OT1	-27.93	-34.95	79.55	15.00
215	MET	OT2	-28.65	-36.17	77.89	15.00
216	HOH	OH2	-26.08	-16.55	83.97	15.00
217	HOH	OH2	-20.53	-32.33	79.43	15.00
218	HOH	OH2	-31.21	-16.22	65.49	15.00
219	HOH	OH2	-30.95	-18.19	68.23	15.00
220	HOH	OH2	-6.96	-10.59	69.84	15.00
221	HOH	OH2	-15.23	-12.63	73.08	15.00
222	HOH	OH2	-34.53	-23.51	69.96	15.00
223	HOH	OH2	-13.78	-33.08	69.63	15.00
224	HOH	OH2	-17.84	-17.71	57.57	15.00
225	HOH	OH2	-24.92	-31.02	61.65	15.00
226	HOH	OH2	-12.76	-8.21	61.82	15.00
227	HOH	OH2	-14.16	-21.69	66.48	15.00
228	HOH	OH2	-44.08	-26.87	48.48	15.00
229	HOH	OH2	-44.49	-35.40	55.40	15.00
230	HOH	OH2	-39.27	-16.80	68.54	15.00
231	HOH	OH2	-24.12	-35.40	48.13	15.00
232	HOH	OH2	-9.62	-25.46	63.42	15.00
233	HOH	OH2	-46.02	-25.14	44.36	15.00
234	HOH	OH2	-27.99	-19.44	61.96	15.00

TABLE IV

235	HOH	OH2	-22.10	-30.02	61.67	15.00
236	HOH	OH2	-27.35	-15.73	71.93	15.00
237	HOH	OH2	-29.19	-17.48	70.74	15.00
238	HOH	OH2	-29.55	-22.69	83.52	15.00
239	HOH	OH2	-35.73	-26.96	51.77	15.00
240	HOH	OH2	-36.27	-24.64	49.31	15.00
241	HOH	OH2	-46.67	-33.01	57.38	15.00
242	HOH	OH2	-27.40	-10.90	68.66	15.00
243	HOH	OH2	-42.01	-15.97	60.76	15.00
244	HOH	OH2	-18.00	-3.18	62.85	15.00
245	HOH	OH2	-33.49	-28.43	70.56	15.00
246	HOH	OH2	-44.87	-25.33	75.86	15.00
247	HOH	OH2	-17.32	-10.85	74.90	15.00
248	HOH	OH2	-11.45	-17.84	66.51	15.00
249	HOH	OH2	-11.56	-21.89	82.27	15.00
250	HOH	OH2	-28.01	-35.21	58.24	15.00
251	HOH	OH2	-35.05	-10.64	53.00	15.00
252	HOH	OH2	-31.64	-28.63	46.10	15.00
253	HOH	OH2	-35.04	-24.79	46.85	15.00
254	HOH	OH2	-41.38	-35.11	55.81	15.00
255	HOH	OH2	-40.44	-19.77	71.52	15.00
256	HOH	OH2	-43.66	-16.34	65.70	15.00
257	HOH	OH2	-39.00	-11.99	70.39	15.00
258	HOH	OH2	-30.92	-9.07	66.51	15.00
259	HOH	OH2	-32.51	-6.89	60.41	15.00
260	HOH	OH2	-19.20	-8.29	62.91	15.00
261	HOH	OH2	-33.67	-20.84	69.78	15.00
262	HOH	OH2	-32.87	-44.92	73.87	15.00
263	HOH	OH2	-13.20	-24.01	76.81	15.00
264	HOH	OH2	-8.83	-25.26	60.26	15.00
265	HOH	OH2	-17.23	-39.22	57.64	15.00
266	HOH	OH2	-21.10	-32.62	61.09	15.00
267	HOH	OH2	-24.50	-33.44	60.85	15.00
268	HOH	OH2	-6.37	-28.13	76.25	15.00
269	HOH	OH2	-10.20	-38.51	65.40	15.00
270	HOH	OH2	-21.41	-37.76	78.27	15.00
271	HOH	OH2	-22.56	-38.95	69.33	15.00
272	HOH	OH2	-30.18	-25.13	93.77	15.00
273	HOH	OH2	-12.08	-12.20	63.63	15.00
274	HOH	OH2	-1.36	-9.62	67.96	15.00
275	HOH	OH2	-28.39	-30.26	56.30	15.00
276	HOH	OH2	-29.74	-20.19	48.42	15.00
277	HOH	OH2	-26.12	-23.01	44.41	15.00

TABLE IV

278	HOH	OH2	-29.92	-34.21	47.42	15.00
279	HOH	OH2	-26.24	-33.39	47.92	15.00
280	HOH	OH2	-32.19	-28.29	42.42	15.00
281	HOH	OH2	-37.49	-30.33	50.55	15.00

TABLE V

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for the cathepsin K complex with inhibitor (1S)-N-[2-[(1-benzyloxycarbonylamino)-3-methylbutyl]thiazol-4-ylcarbonyl]-N'-(N-benzyloxycarbonyl-L-leucinyloxy)hydrazide.

Residue Atom	X	Y	Z	B
1 ALA CB	-44.33	-37.20	63.83	15.00
1 ALA C	-46.76	-36.62	63.83	15.00
1 ALA O	-47.46	-36.94	62.86	15.00
1 ALA N	-46.07	-38.96	63.89	15.00
1 ALA CA	-45.70	-37.59	64.36	15.00
2 PRO N	-46.94	-35.47	64.51	15.00
2 PRO CD	-46.25	-35.02	65.74	15.00
2 PRO CA	-47.93	-34.49	64.07	15.00
2 PRO CB	-47.63	-33.28	64.97	15.00
2 PRO CG	-47.15	-33.90	66.23	15.00
2 PRO C	-47.63	-34.15	62.63	15.00
2 PRO O	-46.50	-34.30	62.16	15.00
3 ASP N	-48.65	-33.74	61.88	15.00
3 ASP CA	-48.39	-33.36	60.52	15.00
3 ASP CB	-49.60	-33.60	59.63	15.00
3 ASP CG	-49.78	-35.10	59.29	15.00
3 ASP OD1	-50.65	-35.42	58.45	15.00
3 ASP OD2	-49.05	-35.95	59.86	15.00
3 ASP C	-47.92	-31.92	60.51	15.00
3 ASP O	-47.44	-31.42	59.49	15.00
4 SER N	-47.94	-31.30	61.69	15.00
4 SER CA	-47.55	-29.91	61.87	15.00
4 SER CB	-48.70	-28.98	61.49	15.00
4 SER OG	-48.42	-27.64	61.85	15.00
4 SER C	-47.13	-29.61	63.29	15.00
4 SER O	-47.79	-30.03	64.24	15.00
5 VAL N	-46.04	-28.86	63.45	15.00
5 VAL CA	-45.60	-28.47	64.78	15.00
5 VAL CB	-44.86	-29.61	65.53	15.00
5 VAL CG1	-43.46	-29.81	64.97	15.00
5 VAL CG2	-44.83	-29.31	67.02	15.00
5 VAL C	-44.78	-27.20	64.70	15.00
5 VAL O	-44.00	-26.98	63.77	15.00

TABLE V

6 ASP N	-44.98	-26.34	65.69	15.00
6 ASP CA	-44.29	-25.07	65.76	15.00
6 ASP CB	-45.27	-23.94	65.39	15.00
6 ASP CG	-44.57	-22.65	65.00	15.00
6 ASP OD1	-43.38	-22.47	65.35	15.00
6 ASP OD2	-45.21	-21.81	64.33	15.00
6 ASP C	-43.72	-24.87	67.16	15.00
6 ASP O	-44.44	-24.51	68.10	15.00
7 TYR N	-42.41	-25.07	67.29	15.00
7 TYR CA	-41.75	-24.90	68.58	15.00
7 TYR CB	-40.35	-25.51	68.57	15.00
7 TYR CG	-40.39	-27.00	68.75	15.00
7 TYR CD1	-40.49	-27.57	70.02	15.00
7 TYR CE1	-40.58	-28.94	70.20	15.00
7 TYR CD2	-40.38	-27.87	67.65	15.00
7 TYR CE2	-40.47	-29.25	67.81	15.00
7 TYR CZ	-40.57	-29.77	69.09	15.00
7 TYR OH	-40.68	-31.13	69.28	15.00
7 TYR C	-41.75	-23.46	69.08	15.00
7 TYR O	-41.62	-23.22	70.29	15.00
8 ARG N	-41.91	-22.51	68.17	15.00
8 ARG CA	-41.98	-21.10	68.55	15.00
8 ARG CB	-42.05	-20.19	67.33	15.00
8 ARG CG	-40.91	-20.36	66.38	15.00
8 ARG CD	-41.09	-19.45	65.19	15.00
8 ARG NE	-42.20	-19.81	64.32	15.00
8 ARG CZ	-42.56	-19.12	63.24	15.00
8 ARG NH1	-41.89	-18.03	62.89	15.00
8 ARG NH2	-43.63	-19.48	62.56	15.00
8 ARG C	-43.22	-20.92	69.42	15.00
8 ARG O	-43.17	-20.22	70.43	15.00
9 LYS N	-44.31	-21.59	69.04	15.00
9 LYS CA	-45.55	-21.53	69.81	15.00
9 LYS CB	-46.77	-21.98	68.99	15.00
9 LYS CG	-47.20	-21.00	67.88	15.00
9 LYS CD	-48.52	-21.46	67.22	15.00
9 LYS CE	-48.99	-20.55	66.08	15.00
9 LYS NZ	-49.38	-19.15	66.49	15.00
9 LYS C	-45.44	-22.32	71.13	15.00
9 LYS O	-46.27	-22.17	72.02	15.00
10 LYS N	-44.41	-23.16	71.23	15.00
10 LYS CA	-44.17	-23.94	72.43	15.00

TABLE V

10	LYS	CB	-43.58	-25.32	72.11	15.00
10	LYS	CG	-44.58	-26.34	71.57	15.00
10	LYS	CD	-43.93	-27.72	71.47	15.00
10	LYS	CE	-44.97	-28.81	71.25	15.00
10	LYS	NZ	-45.93	-28.85	72.39	15.00
10	LYS	C	-43.25	-23.20	73.40	15.00
10	LYS	O	-43.06	-23.65	74.53	15.00
11	GLY	N	-42.67	-22.09	72.95	15.00
11	GLY	CA	-41.78	-21.32	73.79	15.00
11	GLY	C	-40.38	-21.91	73.87	15.00
11	GLY	O	-39.64	-21.67	74.83	15.00
12	TYR	N	-40.01	-22.66	72.84	15.00
12	TYR	CA	-38.71	-23.31	72.77	15.00
12	TYR	CB	-38.80	-24.65	72.05	15.00
12	TYR	CG	-39.27	-25.80	72.87	15.00
12	TYR	CD1	-40.41	-25.71	73.66	15.00
12	TYR	CE1	-40.84	-26.79	74.42	15.00
12	TYR	CD2	-38.57	-27.00	72.85	15.00
12	TYR	CE2	-38.99	-28.09	73.59	15.00
12	TYR	CZ	-40.12	-27.98	74.38	15.00
12	TYR	OH	-40.50	-29.07	75.14	15.00
12	TYR	C	-37.64	-22.48	72.08	15.00
12	TYR	O	-36.46	-22.81	72.16	15.00
13	VAL	N	-38.06	-21.44	71.37	15.00
13	VAL	CA	-37.14	-20.62	70.58	15.00
13	VAL	CB	-37.66	-20.50	69.13	15.00
13	VAL	CG1	-36.66	-19.77	68.25	15.00
13	VAL	CG2	-37.95	-21.87	68.56	15.00
13	VAL	C	-36.89	-19.23	71.14	15.00
13	VAL	O	-37.84	-18.50	71.45	15.00
14	THR	N	-35.63	-18.84	71.23	15.00
14	THR	CA	-35.31	-17.51	71.72	15.00
14	THR	CB	-33.91	-17.47	72.36	15.00
14	THR	OG1	-32.93	-17.77	71.36	15.00
14	THR	CG2	-33.80	-18.49	73.47	15.00
14	THR	C	-35.44	-16.50	70.56	15.00
14	THR	O	-35.63	-16.89	69.40	15.00
15	PRO	N	-35.41	-15.19	70.86	15.00
15	PRO	CD	-35.34	-14.54	72.18	15.00
15	PRO	CA	-35.53	-14.18	69.79	15.00
15	PRO	CB	-35.29	-12.87	70.53	15.00
15	PRO	CG	-35.87	-13.15	71.89	15.00

TABLE V

15 PRO C	-34.52	-14.37	68.66	15.00
15 PRO O	-33.50	-15.04	68.82	15.00
16 VAL N	-34.82	-13.76	67.52	15.00
16 VAL CA	-33.93	-13.83	66.37	15.00
16 VAL CB	-34.62	-13.31	65.09	15.00
16 VAL CG1	-33.61	-13.11	63.98	15.00
16 VAL CG2	-35.68	-14.31	64.65	15.00
16 VAL C	-32.68	-13.01	66.64	15.00
16 VAL O	-32.76	-11.88	67.11	15.00
17 LYS N	-31.52	-13.61	66.39	15.00
17 LYS CA	-30.24	-12.96	66.58	15.00
17 LYS CB	-29.25	-13.89	67.30	15.00
17 LYS CG	-29.81	-14.64	68.50	15.00
17 LYS CD	-30.24	-13.71	69.61	15.00
17 LYS CE	-30.58	-14.46	70.88	15.00
17 LYS NZ	-31.75	-15.34	70.73	15.00
17 LYS C	-29.67	-12.53	65.23	15.00
17 LYS O	-30.20	-12.88	64.17	15.00
18 ASN N	-28.57	-11.79	65.27	15.00
18 ASN CA	-27.90	-11.32	64.06	15.00
18 ASN CB	-28.17	-9.84	63.80	15.00
18 ASN CG	-27.66	-9.39	62.45	15.00
18 ASN OD1	-26.79	-10.02	61.85	15.00
18 ASN ND2	-28.20	-8.29	61.95	15.00
18 ASN C	-26.41	-11.58	64.19	15.00
18 ASN O	-25.74	-11.03	65.08	15.00
19 GLN N	-25.89	-12.42	63.30	15.00
19 GLN CA	-24.48	-12.75	63.31	15.00
19 GLN CB	-24.20	-14.02	62.48	15.00
19 GLN CG	-24.56	-13.94	61.00	15.00
19 GLN CD	-24.28	-15.24	60.27	15.00
19 GLN OE1	-25.14	-15.79	59.60	15.00
19 GLN NE2	-23.06	-15.74	60.40	15.00
19 GLN C	-23.59	-11.60	62.86	15.00
19 GLN O	-22.43	-11.51	63.27	15.00
20 GLY N	-24.12	-10.71	62.03	15.00
20 GLY CA	-23.32	-9.59	61.55	15.00
20 GLY C	-22.33	-10.05	60.49	15.00
20 GLY O	-22.59	-11.03	59.78	15.00
21 GLN N	-21.19	-9.38	60.40	15.00
21 GLN CA	-20.18	-9.73	59.39	15.00
21 GLN CB	-19.51	-8.48	58.81	15.00

TABLE V

21 GLN CG	-20.42	-7.63	57.93	15.00
21 GLN CD	-20.79	-8.33	56.62	15.00
21 GLN OE1	-20.02	-9.12	56.07	15.00
21 GLN NE2	-21.97	-8.02	56.11	15.00
21 GLN C	-19.15	-10.71	59.95	15.00
21 GLN O	-17.96	-10.40	60.02	15.00
22 CYS N	-19.63	-11.88	60.34	15.00
22 CYS CA	-18.79	-12.94	60.89	15.00
22 CYS C	-19.49	-14.24	60.53	15.00
22 CYS O	-20.71	-14.34	60.62	15.00
22 CYS CB	-18.61	-12.78	62.41	15.00
22 CYS SG	-18.03	-14.24	63.33	15.00
23 GLY N	-18.73	-15.19	60.00	15.00
23 GLY CA	-19.29	-16.48	59.66	15.00
23 GLY C	-19.53	-17.35	60.89	15.00
23 GLY O	-19.04	-18.48	60.98	15.00
24 SER N	-20.36	-16.86	61.81	15.00
24 SER CA	-20.67	-17.60	63.03	15.00
24 SER CB	-20.61	-16.66	64.22	15.00
24 SER OG	-21.35	-15.49	63.95	15.00
24 SER C	-22.01	-18.36	62.96	15.00
24 SER O	-22.58	-18.73	63.99	15.00
25 CYS N	-22.50	-18.58	61.74	15.00
25 CYS CA	-23.76	-19.28	61.52	15.00
25 CYS CB	-23.98	-19.51	60.01	15.00
25 CYS SG	-22.57	-20.30	59.15	15.00
25 CYS C	-23.86	-20.58	62.32	15.00
25 CYS O	-24.84	-20.82	63.02	15.00
25 INH C1	-28.50	-9.52	55.70	15.00
25 INH C2	-28.63	-9.33	57.08	15.00
25 INH C3	-27.56	-9.63	57.94	15.00
25 INH C4	-26.35	-10.11	57.43	15.00
25 INH C5	-26.23	-10.29	56.05	15.00
25 INH C6	-27.29	-10.00	55.19	15.00
25 INH C7	-25.20	-10.40	58.35	15.00
25 INH O8	-24.73	-11.77	58.36	15.00
25 INH C9	-24.03	-12.42	57.30	15.00
25 INH O10	-24.33	-12.23	56.10	15.00
25 INH C11	-22.27	-14.01	56.70	15.00
25 INH C12	-20.77	-13.63	56.80	15.00
25 INH C13	-20.18	-12.60	55.82	15.00
25 INH C14	-19.01	-11.83	56.47	15.00

TABLE V

25 INH C15	-21.22	-11.63	55.23	15.00
25 INH C16	-22.50	-15.59	56.80	15.00
25 INH S17	-23.78	-16.32	55.92	15.00
25 INH N18	-21.80	-16.55	57.50	15.00
25 INH C19	-22.21	-17.87	57.39	15.00
25 INH N20	-23.05	-13.25	57.68	15.00
25 INH C21	-23.27	-17.88	56.55	15.00
25 INH C22	-21.58	-19.10	58.24	15.00
25 INH O23	-21.37	-18.39	59.17	15.00
25 INH C24	-13.79	-23.51	54.96	15.00
25 INH C25	-14.23	-22.84	56.08	15.00
25 INH C26	-14.83	-23.54	57.12	15.00
25 INH C27	-15.00	-24.93	57.04	15.00
25 INH C28	-14.54	-25.60	55.91	15.00
25 INH C29	-13.94	-24.90	54.87	15.00
25 INH C30	-15.72	-25.67	58.14	15.00
25 INH O31	-17.10	-25.93	57.71	15.00
25 INH C32	-17.91	-25.03	56.96	15.00
25 INH O33	-17.69	-24.81	55.77	15.00
25 INH C34	-19.82	-23.49	57.00	15.00
25 INH C35	-21.22	-24.12	56.84	15.00
25 INH C36	-21.92	-24.89	57.97	15.00
25 INH C37	-21.43	-26.31	58.12	15.00
25 INH C38	-21.86	-24.15	59.29	15.00
25 INH C39	-19.87	-22.15	57.76	15.00
25 INH O40	-19.60	-22.13	58.96	15.00
25 INH N41	-20.18	-21.00	57.08	15.00
25 INH N42	-20.20	-19.65	57.78	15.00
25 INH N43	-18.90	-24.44	57.63	15.00
26 TRP N	-22.80	-21.38	62.25	15.00
26 TRP CA	-22.73	-22.65	62.97	15.00
26 TRP CB	-21.39	-23.33	62.67	15.00
26 TRP CG	-20.19	-22.46	62.98	15.00
26 TRP CD2	-19.41	-22.45	64.19	15.00
26 TRP CE2	-18.44	-21.44	64.05	15.00
26 TRP CE3	-19.43	-23.21	65.37	15.00
26 TRP CD1	-19.67	-21.48	62.19	15.00
26 TRP NE1	-18.62	-20.86	62.82	15.00
26 TRP CZ2	-17.50	-21.15	65.06	15.00
26 TRP CZ3	-18.50	-22.92	66.37	15.00
26 TRP CH2	-17.55	-21.91	66.21	15.00
26 TRP C	-22.95	-22.50	64.49	15.00

TABLE V

26 TRP O	-23.65	-23.30	65.10	15.00
27 ALA N	-22.35	-21.46	65.08	15.00
27 ALA CA	-22.45	-21.18	66.51	15.00
27 ALA CB	-21.56	-20.02	66.89	15.00
27 ALA C	-23.90	-20.90	66.88	15.00
27 ALA O	-24.46	-21.56	67.74	15.00
28 PHE N	-24.53	-19.94	66.19	15.00
28 PHE CA	-25.93	-19.58	66.41	15.00
28 PHE CB	-26.36	-18.44	65.48	15.00
28 PHE CG	-25.83	-17.09	65.88	15.00
28 PHE CD1	-24.66	-16.59	65.32	15.00
28 PHE CD2	-26.48	-16.32	66.84	15.00
28 PHE CE1	-24.14	-15.37	65.71	15.00
28 PHE CE2	-25.97	-15.09	67.24	15.00
28 PHE CZ	-24.80	-14.62	66.67	15.00
28 PHE C	-26.87	-20.78	66.23	15.00
28 PHE O	-27.85	-20.92	66.96	15.00
29 SER N	-26.56	-21.64	65.26	15.00
29 SER CA	-27.35	-22.83	64.99	15.00
29 SER CB	-26.95	-23.45	63.64	15.00
29 SER OG	-27.63	-24.63	63.36	15.00
29 SER C	-27.21	-23.84	66.13	15.00
29 SER O	-28.19	-24.49	66.50	15.00
30 SER N	-26.01	-23.96	66.69	15.00
30 SER CA	-25.73	-24.88	67.79	15.00
30 SER CB	-24.23	-25.10	68.00	15.00
30 SER OG	-23.60	-25.57	66.82	15.00
30 SER C	-26.37	-24.39	69.09	15.00
30 SER O	-26.95	-25.16	69.85	15.00
31 VAL N	-26.23	-23.09	69.33	15.00
31 VAL CA	-26.80	-22.45	70.51	15.00
31 VAL CB	-26.39	-20.95	70.55	15.00
31 VAL CG1	-27.42	-20.12	71.24	15.00
31 VAL CG2	-25.07	-20.81	71.26	15.00
31 VAL C	-28.31	-22.63	70.48	15.00
31 VAL O	-28.91	-22.92	71.51	15.00
32 GLY N	-28.89	-22.52	69.29	15.00
32 GLY CA	-30.32	-22.68	69.11	15.00
32 GLY C	-30.78	-24.09	69.45	15.00
32 GLY O	-31.86	-24.28	69.99	15.00
33 ALA N	-29.97	-25.08	69.09	15.00
33 ALA CA	-30.29	-26.47	69.38	15.00

TABLE V

33 ALA CB	-29.33	-27.39	68.65	15.00
33 ALA C	-30.19	-26.70	70.89	15.00
33 ALA O	-31.08	-27.30	71.50	15.00
34 LEU N	-29.13	-26.18	71.50	15.00
34 LEU CA	-28.93	-26.32	72.93	15.00
34 LEU CB	-27.58	-25.75	73.35	15.00
34 LEU CG	-26.31	-26.50	72.95	15.00
34 LEU CD1	-25.08	-25.64	73.21	15.00
34 LEU CD2	-26.24	-27.79	73.73	15.00
34 LEU C	-30.07	-25.65	73.69	15.00
34 LEU O	-30.59	-26.21	74.64	15.00
35 GLU N	-30.47	-24.47	73.22	15.00
35 GLU CA	-31.55	-23.70	73.82	15.00
35 GLU CB	-31.77	-22.39	73.08	15.00
35 GLU CG	-30.84	-21.28	73.54	15.00
35 GLU CD	-30.76	-20.13	72.55	15.00
35 GLU OE1	-31.51	-20.14	71.54	15.00
35 GLU OE2	-29.93	-19.22	72.76	15.00
35 GLU C	-32.86	-24.47	73.95	15.00
35 GLU O	-33.52	-24.39	75.00	15.00
36 GLY N	-33.21	-25.21	72.90	15.00
36 GLY CA	-34.42	-26.00	72.90	15.00
36 GLY C	-34.35	-27.13	73.91	15.00
36 GLY O	-35.29	-27.37	74.66	15.00
37 GLN N	-33.22	-27.82	73.95	15.00
37 GLN CA	-33.04	-28.92	74.90	15.00
37 GLN CB	-31.77	-29.71	74.56	15.00
37 GLN CG	-31.84	-30.38	73.19	15.00
37 GLN CD	-33.17	-31.11	72.97	15.00
37 GLN OE1	-33.60	-31.90	73.81	15.00
37 GLN NE2	-33.82	-30.83	71.85	15.00
37 GLN C	-33.05	-28.41	76.35	15.00
37 GLN O	-33.63	-29.04	77.23	15.00
38 LEU N	-32.45	-27.24	76.57	15.00
38 LEU CA	-32.42	-26.63	77.90	15.00
38 LEU CB	-31.61	-25.34	77.89	15.00
38 LEU CG	-31.50	-24.54	79.20	15.00
38 LEU CD1	-30.94	-25.41	80.34	15.00
38 LEU CD2	-30.60	-23.34	78.95	15.00
38 LEU C	-33.85	-26.35	78.35	15.00
38 LEU O	-34.22	-26.60	79.50	15.00
39 LYS N	-34.66	-25.84	77.42	15.00

TABLE V

39 LYS CA	-36.06	-25.56	77.68	15.00
39 LYS CB	-36.71	-24.85	76.49	15.00
39 LYS CG	-38.21	-24.62	76.62	15.00
39 LYS CD	-38.52	-23.64	77.74	15.00
39 LYS CE	-40.03	-23.47	77.92	15.00
39 LYS NZ	-40.35	-22.39	78.91	15.00
39 LYS C	-36.83	-26.83	78.04	15.00
39 LYS O	-37.55	-26.89	79.04	15.00
40 LYS N	-36.65	-27.87	77.23	15.00
40 LYS CA	-37.33	-29.14	77.44	15.00
40 LYS CB	-37.06	-30.09	76.28	15.00
40 LYS CG	-37.54	-31.50	76.53	15.00
40 LYS CD	-37.53	-32.32	75.26	15.00
40 LYS CE	-38.47	-31.72	74.22	15.00
40 LYS NZ	-38.75	-32.66	73.09	15.00
40 LYS C	-37.01	-29.80	78.78	15.00
40 LYS O	-37.92	-30.20	79.52	15.00
41 LYS N	-35.73	-29.90	79.11	15.00
41 LYS CA	-35.29	-30.52	80.36	15.00
41 LYS CB	-33.84	-31.02	80.22	15.00
41 LYS CG	-33.70	-32.50	79.87	15.00
41 LYS CD	-34.49	-32.90	78.62	15.00
41 LYS CE	-33.58	-33.12	77.41	15.00
41 LYS NZ	-33.06	-31.85	76.83	15.00
41 LYS C	-35.47	-29.73	81.68	15.00
41 LYS O	-35.74	-30.32	82.73	15.00
42 THR N	-35.28	-28.40	81.63	15.00
42 THR CA	-35.41	-27.57	82.83	15.00
42 THR CB	-34.17	-26.65	83.04	15.00
42 THR OG1	-34.20	-25.57	82.10	15.00
42 THR CG2	-32.87	-27.43	82.84	15.00
42 THR C	-36.64	-26.66	82.82	15.00
42 THR O	-37.07	-26.16	83.86	15.00
43 GLY N	-37.17	-26.41	81.63	15.00
43 GLY CA	-38.33	-25.55	81.52	15.00
43 GLY C	-37.93	-24.10	81.41	15.00
43 GLY O	-38.78	-23.23	81.26	15.00
44 LYS N	-36.63	-23.82	81.53	15.00
44 LYS CA	-36.11	-22.46	81.41	15.00
44 LYS CB	-34.91	-22.24	82.33	15.00
44 LYS CG	-35.25	-22.15	83.79	15.00
44 LYS CD	-34.06	-21.63	84.59	15.00

TABLE V

44 LYS CE	-33.69	-20.18	84.17	15.00
44 LYS NZ	-32.77	-19.50	85.16	15.00
44 LYS C	-35.72	-22.17	79.96	15.00
44 LYS O	-35.24	-23.05	79.25	15.00
45 LEU N	-35.91	-20.93	79.54	15.00
45 LEU CA	-35.56	-20.52	78.19	15.00
45 LEU CB	-36.80	-20.28	77.31	15.00
45 LEU CG	-36.49	-19.86	75.87	15.00
45 LEU CD1	-36.01	-21.07	75.08	15.00
45 LEU CD2	-37.69	-19.23	75.17	15.00
45 LEU C	-34.71	-19.26	78.25	15.00
45 LEU O	-35.22	-18.17	78.53	15.00
46 LEU N	-33.41	-19.42	78.02	15.00
46 LEU CA	-32.50	-18.29	78.00	15.00
46 LEU CB	-31.75	-18.14	79.35	15.00
46 LEU CG	-31.05	-19.27	80.11	15.00
46 LEU CD1	-32.04	-20.12	80.86	15.00
46 LEU CD2	-30.23	-20.09	79.17	15.00
46 LEU C	-31.54	-18.34	76.80	15.00
46 LEU O	-31.41	-19.37	76.14	15.00
47 ASN N	-30.93	-17.20	76.48	15.00
47 ASN CA	-30.00	-17.12	75.36	15.00
47 ASN CB	-29.88	-15.69	74.84	15.00
47 ASN CG	-31.21	-15.12	74.46	15.00
47 ASN OD1	-31.91	-15.66	73.60	15.00
47 ASN ND2	-31.59	-14.04	75.11	15.00
47 ASN C	-28.64	-17.64	75.75	15.00
47 ASN O	-28.10	-17.24	76.78	15.00
48 LEU N	-28.12	-18.56	74.94	15.00
48 LEU CA	-26.82	-19.15	75.18	15.00
48 LEU CB	-26.80	-20.63	74.80	15.00
48 LEU CG	-27.73	-21.45	75.71	15.00
48 LEU CD1	-27.55	-22.93	75.44	15.00
48 LEU CD2	-27.44	-21.15	77.17	15.00
48 LEU C	-25.73	-18.36	74.47	15.00
48 LEU O	-26.04	-17.44	73.71	15.00
49 SER N	-24.48	-18.72	74.69	15.00
49 SER CA	-23.36	-18.00	74.12	15.00
49 SER CB	-22.27	-17.78	75.18	15.00
49 SER OG	-21.19	-17.01	74.69	15.00
49 SER C	-22.73	-18.50	72.83	15.00
49 SER O	-21.93	-19.43	72.84	15.00

TABLE V

50 PRO N	-23.07	-17.87	71.68	15.00
50 PRO CD	-24.14	-16.88	71.44	15.00
50 PRO CA	-22.47	-18.30	70.42	15.00
50 PRO CB	-23.33	-17.58	69.36	15.00
50 PRO CG	-23.81	-16.35	70.07	15.00
50 PRO C	-21.00	-17.83	70.39	15.00
50 PRO O	-20.15	-18.48	69.77	15.00
51 GLN N	-20.70	-16.73	71.10	15.00
51 GLN CA	-19.34	-16.18	71.19	15.00
51 GLN CB	-19.35	-14.78	71.82	15.00
51 GLN CG	-18.06	-13.96	71.66	15.00
51 GLN CD	-17.76	-13.49	70.22	15.00
51 GLN OE1	-18.60	-12.89	69.54	15.00
51 GLN NE2	-16.54	-13.74	69.77	15.00
51 GLN C	-18.42	-17.16	71.95	15.00
51 GLN O	-17.25	-17.33	71.59	15.00
52 ASN N	-18.98	-17.86	72.94	15.00
52 ASN CA	-18.23	-18.85	73.70	15.00
52 ASN CB	-19.14	-19.54	74.73	15.00
52 ASN CG	-18.40	-20.50	75.66	15.00
52 ASN OD1	-18.99	-21.02	76.61	15.00
52 ASN ND2	-17.11	-20.73	75.41	15.00
52 ASN C	-17.68	-19.86	72.70	15.00
52 ASN O	-16.50	-20.21	72.73	15.00
53 LEU N	-18.55	-20.28	71.78	15.00
53 LEU CA	-18.19	-21.24	70.74	15.00
53 LEU CB	-19.44	-21.79	70.06	15.00
53 LEU CG	-20.11	-23.02	70.67	15.00
53 LEU CD1	-20.05	-22.96	72.19	15.00
53 LEU CD2	-21.55	-23.11	70.17	15.00
53 LEU C	-17.21	-20.66	69.72	15.00
53 LEU O	-16.19	-21.29	69.42	15.00
54 VAL N	-17.51	-19.46	69.21	15.00
54 VAL CA	-16.65	-18.82	68.22	15.00
54 VAL CB	-17.16	-17.39	67.85	15.00
54 VAL CG1	-16.22	-16.73	66.85	15.00
54 VAL CG2	-18.56	-17.47	67.25	15.00
54 VAL C	-15.19	-18.75	68.68	15.00
54 VAL O	-14.28	-19.13	67.94	15.00
55 ASP N	-14.99	-18.33	69.93	15.00
55 ASP CA	-13.65	-18.18	70.52	15.00
55 ASP CB	-13.64	-17.12	71.64	15.00

TABLE V

55 ASP CG	-14.11	-15.73	71.18	15.00
55 ASP OD1	-14.12	-15.43	69.96	15.00
55 ASP OD2	-14.46	-14.93	72.06	15.00
55 ASP C	-12.98	-19.44	71.08	15.00
55 ASP O	-11.75	-19.53	71.15	15.00
56 CYS N	-13.79	-20.43	71.47	15.00
56 CYS CA	-13.26	-21.63	72.12	15.00
56 CYS C	-13.13	-22.97	71.41	15.00
56 CYS O	-12.36	-23.82	71.86	15.00
56 CYS CB	-13.97	-21.81	73.45	15.00
56 CYS SG	-13.91	-20.34	74.55	15.00
57 VAL N	-13.92	-23.20	70.36	15.00
57 VAL CA	-13.85	-24.48	69.64	15.00
57 VAL CB	-15.13	-24.77	68.83	15.00
57 VAL CG1	-15.08	-26.20	68.30	15.00
57 VAL CG2	-16.37	-24.52	69.66	15.00
57 VAL C	-12.67	-24.45	68.68	15.00
57 VAL O	-12.73	-23.82	67.62	15.00
58 SER N	-11.60	-25.15	69.04	15.00
58 SER CA	-10.40	-25.18	68.22	15.00
58 SER CB	-9.19	-25.66	69.02	15.00
58 SER OG	-9.56	-26.66	69.95	15.00
58 SER C	-10.54	-25.93	66.91	15.00
58 SER O	-9.71	-25.75	66.02	15.00
59 GLU N	-11.56	-26.78	66.79	15.00
59 GLU CA	-11.79	-27.55	65.57	15.00
59 GLU CB	-12.53	-28.86	65.84	15.00
59 GLU CG	-11.72	-29.95	66.56	15.00
59 GLU CD	-11.47	-29.63	68.03	15.00
59 GLU OE1	-12.44	-29.48	68.79	15.00
59 GLU OE2	-10.28	-29.54	68.42	15.00
59 GLU C	-12.51	-26.74	64.50	15.00
59 GLU O	-12.45	-27.06	63.32	15.00
60 ASN N	-13.22	-25.69	64.92	15.00
60 ASN CA	-13.91	-24.83	63.98	15.00
60 ASN CB	-15.29	-24.45	64.49	15.00
60 ASN CG	-16.25	-25.62	64.51	15.00
60 ASN OD1	-17.17	-25.66	65.32	15.00
60 ASN ND2	-16.04	-26.59	63.62	15.00
60 ASN C	-13.03	-23.63	63.72	15.00
60 ASN O	-12.01	-23.46	64.39	15.00
61 ASP N	-13.39	-22.81	62.74	15.00

TABLE V

61 ASP CA	-12.56	-21.66	62.39	15.00
61 ASP CB	-12.27	-21.64	60.88	15.00
61 ASP CG	-11.96	-23.05	60.30	15.00
61 ASP OD1	-12.89	-23.70	59.76	15.00
61 ASP OD2	-10.78	-23.50	60.37	15.00
61 ASP C	-13.12	-20.30	62.86	15.00
61 ASP O	-12.75	-19.26	62.32	15.00
62 GLY N	-13.97	-20.31	63.88	15.00
62 GLY CA	-14.54	-19.06	64.36	15.00
62 GLY C	-15.40	-18.39	63.30	15.00
62 GLY O	-16.41	-18.95	62.84	15.00
63 CYS N	-15.00	-17.18	62.90	15.00
63 CYS CA	-15.71	-16.43	61.88	15.00
63 CYS C	-15.44	-16.96	60.47	15.00
63 CYS O	-16.00	-16.47	59.49	15.00
63 CYS CB	-15.39	-14.94	61.97	15.00
63 CYS SG	-16.00	-14.06	63.45	15.00
64 GLY N	-14.57	-17.97	60.38	15.00
64 GLY CA	-14.27	-18.57	59.09	15.00
64 GLY C	-15.01	-19.88	58.84	15.00
64 GLY O	-14.59	-20.68	58.01	15.00
65 GLY N	-16.09	-20.12	59.59	15.00
65 GLY CA	-16.86	-21.34	59.42	15.00
65 GLY C	-16.66	-22.39	60.49	15.00
65 GLY O	-15.77	-22.30	61.34	15.00
66 GLY N	-17.52	-23.40	60.46	15.00
66 GLY CA	-17.44	-24.49	61.42	15.00
66 GLY C	-18.61	-25.44	61.32	15.00
66 GLY O	-19.49	-25.27	60.48	15.00
67 TYR N	-18.62	-26.44	62.18	15.00
67 TYR CA	-19.68	-27.44	62.21	15.00
67 TYR CB	-19.14	-28.83	61.87	15.00
67 TYR CG	-18.68	-28.95	60.44	15.00
67 TYR CD1	-19.58	-29.32	59.44	15.00
67 TYR CE1	-19.18	-29.39	58.11	15.00
67 TYR CD2	-17.37	-28.64	60.07	15.00
67 TYR CE2	-16.96	-28.70	58.75	15.00
67 TYR CZ	-17.88	-29.07	57.77	15.00
67 TYR OH	-17.50	-29.10	56.45	15.00
67 TYR C	-20.36	-27.48	63.56	15.00
67 TYR O	-19.71	-27.30	64.59	15.00
68 MET N	-21.65	-27.77	63.56	15.00

TABLE V

68 MET CA	-22.44	-27.85	64.78	15.00
68 MET CB	-23.93	-28.03	64.44	15.00
68 MET CG	-24.58	-26.86	63.66	15.00
68 MET SD	-24.01	-26.58	61.93	15.00
68 MET CE	-25.23	-27.50	61.01	15.00
68 MET C	-21.91	-28.98	65.68	15.00
68 MET O	-21.68	-28.77	66.87	15.00
69 THR N	-21.68	-30.16	65.08	15.00
69 THR CA	-21.17	-31.32	65.81	15.00
69 THR CB	-20.89	-32.54	64.87	15.00
69 THR OG1	-20.07	-32.14	63.76	15.00
69 THR CG2	-22.20	-33.12	64.35	15.00
69 THR C	-19.91	-31.01	66.64	15.00
69 THR O	-19.80	-31.46	67.78	15.00
70 ASN N	-18.97	-30.25	66.06	15.00
70 ASN CA	-17.74	-29.87	66.77	15.00
70 ASN CB	-16.76	-29.07	65.89	15.00
70 ASN CG	-16.17	-29.89	64.75	15.00
70 ASN OD1	-15.66	-29.34	63.79	15.00
70 ASN ND2	-16.25	-31.20	64.86	15.00
70 ASN C	-18.11	-29.01	67.98	15.00
70 ASN O	-17.57	-29.19	69.08	15.00
71 ALA N	-19.02	-28.07	67.74	15.00
71 ALA CA	-19.50	-27.16	68.77	15.00
71 ALA CB	-20.44	-26.11	68.16	15.00
71 ALA C	-20.20	-27.92	69.91	15.00
71 ALA O	-20.03	-27.59	71.08	15.00
72 PHE N	-20.95	-28.97	69.56	15.00
72 PHE CA	-21.63	-29.82	70.54	15.00
72 PHE CB	-22.65	-30.75	69.86	15.00
72 PHE CG	-23.80	-30.02	69.25	15.00
72 PHE CD1	-24.32	-28.88	69.86	15.00
72 PHE CD2	-24.37	-30.48	68.08	15.00
72 PHE CE1	-25.40	-28.21	69.30	15.00
72 PHE CE2	-25.46	-29.81	67.51	15.00
72 PHE CZ	-25.97	-28.67	68.13	15.00
72 PHE C	-20.64	-30.63	71.36	15.00
72 PHE O	-20.69	-30.66	72.59	15.00
73 GLN N	-19.71	-31.27	70.67	15.00
73 GLN CA	-18.70	-32.08	71.33	15.00
73 GLN CB	-17.83	-32.79	70.31	15.00
73 GLN CG	-16.90	-33.82	70.92	15.00

TABLE V

73 GLN CD	-16.28	-34.73	69.87	15.00
73 GLN OE1	-16.83	-34.92	68.78	15.00
73 GLN NE2	-15.14	-35.30	70.20	15.00
73 GLN C	-17.87	-31.21	72.25	15.00
73 GLN O	-17.49	-31.64	73.33	15.00
74 TYR N	-17.60	-29.98	71.82	15.00
74 TYR CA	-16.83	-29.03	72.62	15.00
74 TYR CB	-16.61	-27.69	71.89	15.00
74 TYR CG	-16.39	-26.51	72.83	15.00
74 TYR CD1	-15.18	-26.35	73.51	15.00
74 TYR CE1	-15.02	-25.35	74.47	15.00
74 TYR CD2	-17.43	-25.63	73.12	15.00
74 TYR CE2	-17.28	-24.64	74.08	15.00
74 TYR CZ	-16.08	-24.50	74.75	15.00
74 TYR OH	-15.96	-23.57	75.75	15.00
74 TYR C	-17.55	-28.79	73.94	15.00
74 TYR O	-16.92	-28.75	75.00	15.00
75 VAL N	-18.87	-28.62	73.86	15.00
75 VAL CA	-19.70	-28.36	75.04	15.00
75 VAL CB	-21.11	-27.88	74.63	15.00
75 VAL CG1	-21.96	-27.66	75.85	15.00
75 VAL CG2	-21.00	-26.57	73.83	15.00
75 VAL C	-19.77	-29.55	75.98	15.00
75 VAL O	-19.91	-29.38	77.19	15.00
76 GLN N	-19.66	-30.74	75.42	15.00
76 GLN CA	-19.66	-31.95	76.22	15.00
76 GLN CB	-19.84	-33.21	75.36	15.00
76 GLN CG	-19.80	-34.51	76.14	15.00
76 GLN CD	-19.78	-35.75	75.25	15.00
76 GLN OE1	-19.34	-35.70	74.09	15.00
76 GLN NE2	-20.24	-36.86	75.79	15.00
76 GLN C	-18.34	-32.00	77.00	15.00
76 GLN O	-18.34	-32.09	78.22	15.00
77 LYS N	-17.22	-31.90	76.29	15.00
77 LYS CA	-15.89	-31.95	76.91	15.00
77 LYS CB	-14.79	-32.01	75.85	15.00
77 LYS CG	-14.77	-33.29	75.01	15.00
77 LYS CD	-13.80	-33.14	73.84	15.00
77 LYS CE	-13.62	-34.44	73.09	15.00
77 LYS NZ	-12.55	-34.33	72.06	15.00
77 LYS C	-15.63	-30.80	77.87	15.00
77 LYS O	-14.99	-30.98	78.91	15.00

TABLE V

78 ASN N	-16.09	-29.61	77.50	15.00
78 ASN CA	-15.91	-28.43	78.32	15.00
78 ASN CB	-16.18	-27.16	77.51	15.00
78 ASN CG	-15.95	-25.89	78.31	15.00
78 ASN OD1	-14.90	-25.69	78.92	15.00
78 ASN ND2	-16.93	-24.99	78.28	15.00
78 ASN C	-16.83	-28.52	79.52	15.00
78 ASN O	-16.64	-27.81	80.49	15.00
79 ARG N	-17.81	-29.42	79.44	15.00
79 ARG CA	-18.82	-29.64	80.47	15.00
79 ARG CB	-18.19	-30.06	81.81	15.00
79 ARG CG	-17.69	-31.48	81.85	15.00
79 ARG CD	-16.75	-31.70	83.00	15.00
79 ARG NE	-16.07	-32.98	82.88	15.00
79 ARG CZ	-14.79	-33.13	82.56	15.00
79 ARG NH1	-14.02	-32.08	82.33	15.00
79 ARG NH2	-14.28	-34.36	82.41	15.00
79 ARG C	-19.77	-28.45	80.65	15.00
79 ARG O	-20.43	-28.32	81.69	15.00
80 GLY N	-19.84	-27.58	79.66	15.00
80 GLY CA	-20.72	-26.45	79.77	15.00
80 GLY C	-20.50	-25.38	78.73	15.00
80 GLY O	-19.60	-25.49	77.89	15.00
81 ILE N	-21.38	-24.39	78.75	15.00
81 ILE CA	-21.34	-23.24	77.85	15.00
81 ILE CB	-22.12	-23.47	76.52	15.00
81 ILE CG2	-23.54	-24.00	76.80	15.00
81 ILE CG1	-22.15	-22.16	75.71	15.00
81 ILE CD1	-22.81	-22.28	74.36	15.00
81 ILE C	-21.98	-22.09	78.60	15.00
81 ILE O	-23.00	-22.26	79.29	15.00
82 ASP N	-21.37	-20.92	78.48	15.00
82 ASP CA	-21.88	-19.75	79.15	15.00
82 ASP CB	-20.83	-18.66	79.19	15.00
82 ASP CG	-19.68	-19.00	80.10	15.00
82 ASP OD1	-18.57	-18.52	79.85	15.00
82 ASP OD2	-19.91	-19.76	81.07	15.00
82 ASP C	-23.17	-19.21	78.57	15.00
82 ASP O	-23.56	-19.54	77.45	15.00
83 SER N	-23.85	-18.42	79.39	15.00
83 SER CA	-25.09	-17.77	79.00	15.00
83 SER CB	-25.89	-17.34	80.22	15.00

TABLE V

83	SER OG	-25.29	-16.22	80.86	15.00
83	SER C	-24.70	-16.56	78.16	15.00
83	SER O	-23.58	-16.04	78.30	15.00
84	GLU N	-25.59	-16.10	77.30	15.00
84	GLU CA	-25.30	-14.93	76.49	15.00
84	GLU CB	-26.55	-14.46	75.73	15.00
84	GLU CG	-26.40	-13.12	75.04	15.00
84	GLU CD	-25.37	-13.12	73.92	15.00
84	GLU OE1	-24.73	-12.07	73.72	15.00
84	GLU OE2	-25.20	-14.15	73.23	15.00
84	GLU C	-24.74	-13.81	77.37	15.00
84	GLU O	-23.72	-13.20	77.06	15.00
85	ASP N	-25.37	-13.60	78.53	15.00
85	ASP CA	-24.94	-12.54	79.44	15.00
85	ASP CB	-25.85	-12.44	80.66	15.00
85	ASP CG	-27.22	-11.88	80.32	15.00
85	ASP OD1	-28.19	-12.27	81.01	15.00
85	ASP OD2	-27.33	-11.06	79.37	15.00
85	ASP C	-23.49	-12.60	79.87	15.00
85	ASP O	-22.78	-11.59	79.79	15.00
86	ALA N	-23.05	-13.79	80.28	15.00
86	ALA CA	-21.67	-14.00	80.73	15.00
86	ALA CB	-21.59	-15.24	81.59	15.00
86	ALA C	-20.61	-14.06	79.62	15.00
86	ALA O	-19.42	-14.18	79.92	15.00
87	TYR N	-21.04	-13.98	78.36	15.00
87	TYR CA	-20.13	-14.04	77.22	15.00
87	TYR CB	-19.69	-15.50	76.99	15.00
87	TYR CG	-18.30	-15.71	76.41	15.00
87	TYR CD1	-17.79	-14.89	75.41	15.00
87	TYR CE1	-16.54	-15.12	74.86	15.00
87	TYR CD2	-17.51	-16.78	76.84	15.00
87	TYR CE2	-16.26	-17.02	76.29	15.00
87	TYR CZ	-15.78	-16.18	75.30	15.00
87	TYR OH	-14.54	-16.42	74.76	15.00
87	TYR C	-20.88	-13.46	76.00	15.00
87	TYR O	-21.14	-14.15	75.02	15.00
88	PRO N	-21.17	-12.14	76.05	15.00
88	PRO CD	-20.72	-11.16	77.06	15.00
88	PRO CA	-21.90	-11.45	74.97	15.00
88	PRO CB	-21.94	-9.99	75.46	15.00
88	PRO CG	-20.72	-9.87	76.27	15.00

TABLE V

88 PRO C	-21.30	-11.57	73.58	15.00
88 PRO O	-20.11	-11.80	73.42	15.00
89 TYR N	-22.15	-11.39	72.58	15.00
89 TYR CA	-21.74	-11.48	71.18	15.00
89 TYR CB	-22.93	-11.78	70.27	15.00
89 TYR CG	-22.53	-12.08	68.84	15.00
89 TYR CD1	-21.82	-13.23	68.54	15.00
89 TYR CE1	-21.40	-13.50	67.25	15.00
89 TYR CD2	-22.83	-11.20	67.81	15.00
89 TYR CE2	-22.40	-11.46	66.50	15.00
89 TYR CZ	-21.69	-12.62	66.24	15.00
89 TYR OH	-21.23	-12.90	64.98	15.00
89 TYR C	-21.04	-10.21	70.71	15.00
89 TYR O	-21.54	-9.11	70.94	15.00
90 VAL N	-19.88	-10.36	70.08	15.00
90 VAL CA	-19.15	-9.21	69.55	15.00
90 VAL CB	-17.81	-8.94	70.27	15.00
90 VAL CG1	-18.06	-8.15	71.55	15.00
90 VAL CG2	-17.08	-10.23	70.56	15.00
90 VAL C	-18.92	-9.31	68.05	15.00
90 VAL O	-18.60	-8.32	67.40	15.00
91 GLY N	-19.08	-10.51	67.50	15.00
91 GLY CA	-18.90	-10.68	66.06	15.00
91 GLY C	-17.46	-10.67	65.56	15.00
91 GLY O	-17.19	-10.28	64.42	15.00
92 GLN N	-16.54	-11.10	66.41	15.00
92 GLN CA	-15.14	-11.17	66.04	15.00
92 GLN CB	-14.46	-9.80	66.11	15.00
92 GLN CG	-14.41	-9.16	67.49	15.00
92 GLN CD	-14.16	-7.65	67.45	15.00
92 GLN OE1	-14.60	-6.91	68.33	15.00
92 GLN NE2	-13.46	-7.18	66.42	15.00
92 GLN C	-14.45	-12.22	66.92	15.00
92 GLN O	-14.82	-12.42	68.07	15.00
93 GLU N	-13.51	-12.94	66.32	15.00
93 GLU CA	-12.75	-13.98	66.99	15.00
93 GLU CB	-11.92	-14.80	65.98	15.00
93 GLU CG	-12.60	-15.10	64.64	15.00
93 GLU CD	-11.66	-15.74	63.60	15.00
93 GLU OE1	-10.42	-15.60	63.72	15.00
93 GLU OE2	-12.17	-16.37	62.65	15.00
93 GLU C	-11.83	-13.34	68.03	15.00

TABLE V

93	GLU O	-11.21	-12.30	67.75	15.00
94	GLU N	-11.73	-13.97	69.20	15.00
94	GLU CA	-10.88	-13.49	70.30	15.00
94	GLU CB	-11.58	-12.42	71.15	15.00
94	GLU CG	-11.71	-11.07	70.44	15.00
94	GLU CD	-12.53	-10.04	71.21	15.00
94	GLU OE1	-13.43	-10.42	71.98	15.00
94	GLU OE2	-12.26	-8.84	71.02	15.00
94	GLU C	-10.47	-14.70	71.15	15.00
94	GLU O	-10.92	-15.82	70.89	15.00
95	SER N	-9.61	-14.49	72.13	15.00
95	SER CA	-9.17	-15.58	72.99	15.00
95	SER CB	-7.98	-15.16	73.87	15.00
95	SER OG	-8.29	-14.05	74.70	15.00
95	SER C	-10.29	-16.20	73.83	15.00
95	SER O	-11.16	-15.50	74.36	15.00
96	CYS N	-10.27	-17.53	73.93	15.00
96	CYS CA	-11.26	-18.23	74.72	15.00
96	CYS C	-11.28	-17.62	76.13	15.00
96	CYS O	-10.26	-17.58	76.83	15.00
96	CYS CB	-10.97	-19.73	74.75	15.00
96	CYS SG	-12.23	-20.69	75.64	15.00
97	MET N	-12.44	-17.08	76.50	15.00
97	MET CA	-12.64	-16.44	77.80	15.00
97	MET CB	-12.80	-14.93	77.61	15.00
97	MET CG	-12.60	-14.11	78.87	15.00
97	MET SD	-10.92	-14.28	79.50	15.00
97	MET CE	-10.06	-13.18	78.42	15.00
97	MET C	-13.84	-17.05	78.53	15.00
97	MET O	-14.64	-16.34	79.14	15.00
98	TYR N	-13.96	-18.37	78.44	15.00
98	TYR CA	-15.04	-19.09	79.10	15.00
98	TYR CB	-15.03	-20.57	78.73	15.00
98	TYR CG	-15.99	-21.40	79.55	15.00
98	TYR CD1	-17.36	-21.36	79.31	15.00
98	TYR CE1	-18.25	-22.09	80.09	15.00
98	TYR CD2	-15.53	-22.21	80.59	15.00
98	TYR CE2	-16.41	-22.95	81.38	15.00
98	TYR CZ	-17.77	-22.88	81.13	15.00
98	TYR OH	-18.64	-23.57	81.93	15.00
98	TYR C	-15.01	-18.91	80.61	15.00
98	TYR O	-14.00	-19.18	81.26	15.00

TABLE V

99 ASN N	-16.12	-18.44	81.16	15.00
99 ASN CA	-16.24	-18.23	82.58	15.00
99 ASN CB	-16.80	-16.84	82.89	15.00
99 ASN CG	-16.73	-16.50	84.38	15.00
99 ASN OD1	-16.91	-17.36	85.24	15.00
99 ASN ND2	-16.44	-15.25	84.68	15.00
99 ASN C	-17.14	-19.31	83.15	15.00
99 ASN O	-18.33	-19.37	82.85	15.00
100 PRO N	-16.59	-20.19	83.99	15.00
100 PRO CD	-15.16	-20.25	84.37	15.00
100 PRO CA	-17.34	-21.29	84.62	15.00
100 PRO CB	-16.27	-21.98	85.47	15.00
100 PRO CG	-15.00	-21.70	84.70	15.00
100 PRO C	-18.52	-20.82	85.48	15.00
100 PRO O	-19.53	-21.51	85.58	15.00
101 THR N	-18.37	-19.64	86.09	15.00
101 THR CA	-19.42	-19.05	86.93	15.00
101 THR CB	-18.92	-17.73	87.61	15.00
101 THR OG1	-17.73	-17.97	88.38	15.00
101 THR CG2	-19.99	-17.15	88.54	15.00
101 THR C	-20.68	-18.73	86.12	15.00
101 THR O	-21.77	-18.69	86.68	15.00
102 GLY N	-20.52	-18.51	84.81	15.00
102 GLY CA	-21.67	-18.18	83.97	15.00
102 GLY C	-22.36	-19.33	83.25	15.00
102 GLY O	-23.34	-19.12	82.53	15.00
103 LYS N	-21.87	-20.54	83.47	15.00
103 LYS CA	-22.41	-21.74	82.83	15.00
103 LYS CB	-21.73	-22.98	83.40	15.00
103 LYS CG	-21.93	-24.24	82.59	15.00
103 LYS CD	-21.93	-25.43	83.52	15.00
103 LYS CE	-20.80	-25.36	84.52	15.00
103 LYS NZ	-21.18	-26.01	85.80	15.00
103 LYS C	-23.91	-21.86	82.95	15.00
103 LYS O	-24.44	-21.97	84.05	15.00
104 ALA N	-24.60	-21.92	81.82	15.00
104 ALA CA	-26.05	-22.02	81.81	15.00
104 ALA CB	-26.65	-20.90	80.97	15.00
104 ALA C	-26.59	-23.38	81.35	15.00
104 ALA O	-27.77	-23.67	81.53	15.00
105 ALA N	-25.72	-24.20	80.77	15.00
105 ALA CA	-26.11	-25.53	80.29	15.00

TABLE V

105 ALA CB	-27.03	-25.41	79.07	15.00
105 ALA C	-24.88	-26.34	79.91	15.00
105 ALA O	-23.75	-25.83	79.94	15.00
106 LYS N	-25.12	-27.60	79.57	15.00
106 LYS CA	-24.10	-28.54	79.11	15.00
106 LYS CB	-23.33	-29.21	80.26	15.00
106 LYS CG	-24.14	-30.16	81.14	15.00
106 LYS CD	-23.57	-31.59	81.11	15.00
106 LYS CE	-24.32	-32.54	82.06	15.00
106 LYS NZ	-25.78	-32.68	81.70	15.00
106 LYS C	-24.83	-29.57	78.27	15.00
106 LYS O	-26.05	-29.54	78.19	15.00
107 CYS N	-24.09	-30.44	77.60	15.00
107 CYS CA	-24.70	-31.48	76.79	15.00
107 CYS CB	-24.95	-31.05	75.34	15.00
107 CYS SG	-23.54	-31.08	74.19	15.00
107 CYS C	-23.84	-32.72	76.88	15.00
107 CYS O	-22.66	-32.64	77.19	15.00
108 ARG N	-24.45	-33.87	76.68	15.00
108 ARG CA	-23.73	-35.13	76.74	15.00
108 ARG CB	-24.36	-36.04	77.78	15.00
108 ARG CG	-24.14	-35.57	79.21	15.00
108 ARG CD	-24.54	-36.64	80.19	15.00
108 ARG NE	-25.96	-36.93	80.10	15.00
108 ARG CZ	-26.54	-38.01	80.61	15.00
108 ARG NH1	-25.81	-38.91	81.24	15.00
108 ARG NH2	-27.85	-38.18	80.50	15.00
108 ARG C	-23.58	-35.82	75.39	15.00
108 ARG O	-23.92	-36.99	75.24	15.00
109 GLY N	-23.09	-35.08	74.41	15.00
109 GLY CA	-22.90	-35.66	73.10	15.00
109 GLY C	-23.96	-35.21	72.13	15.00
109 GLY O	-24.80	-34.38	72.48	15.00
110 TYR N	-23.95	-35.79	70.94	15.00
110 TYR CA	-24.90	-35.45	69.88	15.00
110 TYR CB	-24.35	-34.33	68.98	15.00
110 TYR CG	-23.08	-34.72	68.26	15.00
110 TYR CD1	-21.84	-34.52	68.86	15.00
110 TYR CE1	-20.69	-34.96	68.26	15.00
110 TYR CD2	-23.13	-35.37	67.04	15.00
110 TYR CE2	-21.98	-35.82	66.43	15.00
110 TYR CZ	-20.76	-35.62	67.05	15.00

TABLE V

110 TYR OH	-19.61	-36.09	66.45	15.00
110 TYR C	-25.28	-36.66	69.02	15.00
110 TYR O	-24.66	-37.72	69.09	15.00
111 ARG N	-26.28	-36.45	68.18	15.00
111 ARG CA	-26.77	-37.47	67.27	15.00
111 ARG CB	-28.06	-38.10	67.78	15.00
111 ARG CG	-29.00	-38.71	66.72	15.00
111 ARG CD	-28.59	-40.10	66.19	15.00
111 ARG NE	-29.56	-40.59	65.20	15.00
111 ARG CZ	-29.24	-41.12	64.02	15.00
111 ARG NH1	-27.97	-41.25	63.65	15.00
111 ARG NH2	-30.20	-41.45	63.15	15.00
111 ARG C	-26.95	-36.78	65.92	15.00
111 ARG O	-27.32	-35.60	65.85	15.00
112 GLU N	-26.60	-37.49	64.86	15.00
112 GLU CA	-26.73	-36.98	63.50	15.00
112 GLU CB	-25.44	-37.25	62.71	15.00
112 GLU CG	-24.23	-36.54	63.29	15.00
112 GLU CD	-22.94	-36.81	62.52	15.00
112 GLU OE1	-22.55	-36.00	61.66	15.00
112 GLU OE2	-22.30	-37.84	62.82	15.00
112 GLU C	-27.95	-37.64	62.84	15.00
112 GLU O	-28.32	-38.74	63.20	15.00
113 ILE N	-28.60	-36.94	61.93	15.00
113 ILE CA	-29.75	-37.51	61.24	15.00
113 ILE CB	-30.79	-36.40	60.90	15.00
113 ILE CG2	-31.82	-36.90	59.89	15.00
113 ILE CG1	-31.47	-35.89	62.17	15.00
113 ILE CD1	-32.11	-36.98	63.00	15.00
113 ILE C	-29.23	-38.17	59.97	15.00
113 ILE O	-28.24	-37.70	59.39	15.00
114 PRO N	-29.81	-39.32	59.56	15.00
114 PRO CD	-30.91	-40.08	60.16	15.00
114 PRO CA	-29.34	-39.97	58.34	15.00
114 PRO CB	-30.43	-41.01	58.08	15.00
114 PRO CG	-30.84	-41.40	59.42	15.00
114 PRO C	-29.30	-38.94	57.22	15.00
114 PRO O	-30.29	-38.23	56.97	15.00
115 GLU N	-28.14	-38.81	56.59	15.00
115 GLU CA	-27.95	-37.85	55.52	15.00
115 GLU CB	-26.52	-37.88	55.00	15.00
115 GLU CG	-26.24	-36.84	53.95	15.00

TABLE V

115 GLU CD	-24.87	-36.97	53.34	15.00
115 GLU OE1	-24.73	-37.74	52.35	15.00
115 GLU OE2	-23.94	-36.29	53.84	15.00
115 GLU C	-28.94	-38.05	54.38	15.00
115 GLU O	-29.14	-39.17	53.91	15.00
116 GLY N	-29.55	-36.96	53.95	15.00
116 GLY CA	-30.51	-37.02	52.86	15.00
116 GLY C	-31.93	-37.43	53.23	15.00
116 GLY O	-32.85	-37.23	52.44	15.00
117 ASN N	-32.12	-37.92	54.46	15.00
117 ASN CA	-33.43	-38.37	54.93	15.00
117 ASN CB	-33.27	-39.59	55.85	15.00
117 ASN CG	-34.53	-40.48	55.92	15.00
117 ASN OD1	-35.65	-40.02	55.70	15.00
117 ASN ND2	-34.34	-41.74	56.27	15.00
117 ASN C	-34.30	-37.30	55.60	15.00
117 ASN O	-34.12	-37.00	56.79	15.00
118 GLU N	-35.26	-36.75	54.86	15.00
118 GLU CA	-36.18	-35.73	55.38	15.00
118 GLU CB	-36.91	-34.98	54.26	15.00
118 GLU CG	-36.01	-34.11	53.37	15.00
118 GLU CD	-36.78	-33.09	52.55	15.00
118 GLU OE1	-36.86	-33.26	51.32	15.00
118 GLU OE2	-37.30	-32.11	53.13	15.00
118 GLU C	-37.19	-36.37	56.35	15.00
118 GLU O	-37.57	-35.76	57.35	15.00
119 LYS N	-37.59	-37.60	56.06	15.00
119 LYS CA	-38.53	-38.31	56.92	15.00
119 LYS CB	-38.89	-39.68	56.33	15.00
119 LYS CG	-40.10	-40.36	56.97	15.00
119 LYS CD	-40.37	-41.75	56.35	15.00
119 LYS CE	-39.71	-42.89	57.16	15.00
119 LYS NZ	-39.80	-44.23	56.47	15.00
119 LYS C	-37.89	-38.45	58.30	15.00
119 LYS O	-38.53	-38.23	59.33	15.00
120 ALA N	-36.59	-38.76	58.30	15.00
120 ALA CA	-35.85	-38.91	59.54	15.00
120 ALA CB	-34.44	-39.41	59.25	15.00
120 ALA C	-35.78	-37.58	60.26	15.00
120 ALA O	-35.89	-37.52	61.49	15.00
121 LEU N	-35.61	-36.51	59.48	15.00
121 LEU CA	-35.52	-35.16	60.02	15.00

TABLE V

121 LEU CB	-35.02	-34.18	58.94	15.00
121 LEU CG	-34.84	-32.68	59.23	15.00
121 LEU CD1	-33.98	-32.43	60.46	15.00
121 LEU CD2	-34.25	-32.02	57.99	15.00
121 LEU C	-36.83	-34.68	60.68	15.00
121 LEU O	-36.79	-34.05	61.74	15.00
122 LYS N	-37.97	-35.03	60.08	15.00
122 LYS CA	-39.29	-34.65	60.60	15.00
122 LYS CB	-40.42	-34.99	59.63	15.00
122 LYS CG	-41.82	-34.90	60.26	15.00
122 LYS CD	-42.89	-35.49	59.34	15.00
122 LYS CE	-44.28	-35.44	59.97	15.00
122 LYS NZ	-45.36	-35.91	59.03	15.00
122 LYS C	-39.57	-35.33	61.92	15.00
122 LYS O	-40.03	-34.70	62.88	15.00
123 ARG N	-39.33	-36.63	61.96	15.00
123 ARG CA	-39.55	-37.40	63.17	15.00
123 ARG CB	-39.26	-38.88	62.91	15.00
123 ARG CG	-40.26	-39.53	61.95	15.00
123 ARG CD	-40.04	-41.04	61.79	15.00
123 ARG NE	-38.71	-41.35	61.25	15.00
123 ARG CZ	-37.76	-42.03	61.89	15.00
123 ARG NH1	-37.99	-42.51	63.12	15.00
123 ARG NH2	-36.57	-42.20	61.33	15.00
123 ARG C	-38.72	-36.82	64.33	15.00
123 ARG O	-39.21	-36.72	65.46	15.00
124 ALA N	-37.50	-36.38	64.04	15.00
124 ALA CA	-36.62	-35.79	65.05	15.00
124 ALA CB	-35.21	-35.60	64.50	15.00
124 ALA C	-37.17	-34.46	65.58	15.00
124 ALA O	-37.17	-34.21	66.79	15.00
125 VAL N	-37.64	-33.61	64.68	15.00
125 VAL CA	-38.20	-32.33	65.09	15.00
125 VAL CB	-38.57	-31.44	63.87	15.00
125 VAL CG1	-39.39	-30.23	64.31	15.00
125 VAL CG2	-37.30	-30.97	63.15	15.00
125 VAL C	-39.41	-32.57	65.99	15.00
125 VAL O	-39.53	-31.99	67.07	15.00
126 ALA N	-40.27	-33.49	65.58	15.00
126 ALA CA	-41.46	-33.83	66.34	15.00
126 ALA CB	-42.27	-34.90	65.62	15.00
126 ALA C	-41.15	-34.29	67.77	15.00

TABLE V

126 ALA O	-41.69	-33.74	68.73	15.00
127 ARG N	-40.26	-35.26	67.93	15.00
127 ARG CA	-39.95	-35.76	69.27	15.00
127 ARG CB	-39.99	-37.28	69.30	15.00
127 ARG CG	-38.95	-37.98	68.45	15.00
127 ARG CD	-39.08	-39.48	68.63	15.00
127 ARG NE	-40.43	-39.95	68.30	15.00
127 ARG CZ	-41.25	-40.58	69.14	15.00
127 ARG NH1	-42.47	-40.94	68.73	15.00
127 ARG NH2	-40.88	-40.83	70.39	15.00
127 ARG C	-38.72	-35.26	70.01	15.00
127 ARG O	-38.50	-35.65	71.15	15.00
128 VAL N	-37.91	-34.42	69.40	15.00
128 VAL CA	-36.72	-33.94	70.07	15.00
128 VAL CB	-35.46	-34.31	69.27	15.00
128 VAL CG1	-34.25	-33.52	69.74	15.00
128 VAL CG2	-35.18	-35.79	69.42	15.00
128 VAL C	-36.78	-32.43	70.32	15.00
128 VAL O	-36.54	-31.96	71.43	15.00
129 GLY N	-37.12	-31.68	69.28	15.00
129 GLY CA	-37.18	-30.24	69.39	15.00
129 GLY C	-36.41	-29.69	68.22	15.00
129 GLY O	-36.10	-30.46	67.30	15.00
130 PRO N	-36.09	-28.39	68.19	15.00
130 PRO CD	-36.46	-27.40	69.22	15.00
130 PRO CA	-35.34	-27.75	67.11	15.00
130 PRO CB	-35.01	-26.38	67.70	15.00
130 PRO CG	-36.23	-26.08	68.51	15.00
130 PRO C	-34.06	-28.52	66.73	15.00
130 PRO O	-33.35	-29.05	67.61	15.00
131 VAL N	-33.78	-28.58	65.44	15.00
131 VAL CA	-32.61	-29.30	64.92	15.00
131 VAL CB	-33.05	-30.57	64.15	15.00
131 VAL CG1	-31.85	-31.31	63.57	15.00
131 VAL CG2	-33.84	-31.50	65.07	15.00
131 VAL C	-31.71	-28.42	64.02	15.00
131 VAL O	-32.21	-27.71	63.14	15.00
132 SER N	-30.41	-28.44	64.29	15.00
132 SER CA	-29.40	-27.69	63.53	15.00
132 SER CB	-28.07	-27.65	64.28	15.00
132 SER OG	-28.22	-27.17	65.59	15.00
132 SER C	-29.19	-28.31	62.13	15.00

TABLE V

132 SER O	-28.82	-29.48	62.02	15.00
133 VAL N	-29.40	-27.52	61.08	15.00
133 VAL CA	-29.23	-28.02	59.73	15.00
133 VAL CB	-30.60	-28.18	58.99	15.00
133 VAL CG1	-31.53	-29.06	59.80	15.00
133 VAL CG2	-31.24	-26.84	58.70	15.00
133 VAL C	-28.35	-27.10	58.89	15.00
133 VAL O	-28.22	-25.92	59.20	15.00
134 ALA N	-27.74	-27.66	57.85	15.00
134 ALA CA	-26.88	-26.90	56.95	15.00
134 ALA CB	-25.50	-27.56	56.83	15.00
134 ALA C	-27.59	-26.86	55.59	15.00
134 ALA O	-28.15	-27.87	55.15	15.00
135 ILE N	-27.61	-25.69	54.96	15.00
135 ILE CA	-28.28	-25.52	53.68	15.00
135 ILE CB	-29.64	-24.75	53.86	15.00
135 ILE CG2	-30.59	-25.51	54.77	15.00
135 ILE CG1	-29.37	-23.34	54.39	15.00
135 ILE CD1	-30.61	-22.47	54.50	15.00
135 ILE C	-27.45	-24.69	52.71	15.00
135 ILE O	-26.36	-24.22	53.04	15.00
136 ASP N	-27.98	-24.56	51.49	15.00
136 ASP CA	-27.37	-23.75	50.45	15.00
136 ASP CB	-27.45	-24.42	49.07	15.00
136 ASP CG	-26.86	-23.57	47.94	15.00
136 ASP OD1	-26.91	-24.02	46.79	15.00
136 ASP OD2	-26.35	-22.45	48.19	15.00
136 ASP C	-28.21	-22.46	50.50	15.00
136 ASP O	-29.41	-22.48	50.22	15.00
137 ALA N	-27.58	-21.38	50.92	15.00
137 ALA CA	-28.23	-20.08	51.04	15.00
137 ALA CB	-28.30	-19.68	52.49	15.00
137 ALA C	-27.45	-19.04	50.25	15.00
137 ALA O	-27.31	-17.91	50.69	15.00
138 SER N	-26.97	-19.44	49.08	15.00
138 SER CA	-26.18	-18.56	48.22	15.00
138 SER CB	-25.05	-19.36	47.56	15.00
138 SER OG	-25.57	-20.33	46.67	15.00
138 SER C	-26.99	-17.81	47.16	15.00
138 SER O	-26.48	-16.88	46.52	15.00
139 LEU N	-28.23	-18.24	46.97	15.00
139 LEU CA	-29.11	-17.68	45.97	15.00

TABLE V

139	LEU	CB	-30.17	-18.70	45.55	15.00
139	LEU	CG	-29.68	-19.89	44.71	15.00
139	LEU	CD1	-28.41	-20.51	45.27	15.00
139	LEU	CD2	-30.78	-20.93	44.65	15.00
139	LEU	C	-29.76	-16.35	46.31	15.00
139	LEU	O	-30.20	-16.13	47.44	15.00
140	THR	N	-29.82	-15.48	45.31	15.00
140	THR	CA	-30.41	-14.15	45.44	15.00
140	THR	CB	-30.31	-13.40	44.07	15.00
140	THR	OG1	-28.94	-13.06	43.81	15.00
140	THR	CG2	-31.17	-12.14	44.06	15.00
140	THR	C	-31.87	-14.27	45.91	15.00
140	THR	O	-32.36	-13.41	46.66	15.00
141	SER	N	-32.55	-15.34	45.50	15.00
141	SER	CA	-33.93	-15.58	45.89	15.00
141	SER	CB	-34.47	-16.84	45.23	15.00
141	SER	OG	-33.61	-17.94	45.44	15.00
141	SER	C	-34.00	-15.70	47.41	15.00
141	SER	O	-34.83	-15.07	48.07	15.00
142	PHE	N	-33.07	-16.47	47.97	15.00
142	PHE	CA	-32.99	-16.70	49.40	15.00
142	PHE	CB	-31.94	-17.76	49.73	15.00
142	PHE	CG	-31.90	-18.15	51.17	15.00
142	PHE	CD1	-32.77	-19.12	51.66	15.00
142	PHE	CD2	-31.02	-17.55	52.05	15.00
142	PHE	CE1	-32.75	-19.48	53.00	15.00
142	PHE	CE2	-31.00	-17.90	53.39	15.00
142	PHE	CZ	-31.86	-18.87	53.86	15.00
142	PHE	C	-32.73	-15.42	50.16	15.00
142	PHE	O	-33.46	-15.07	51.08	15.00
143	GLN	N	-31.67	-14.71	49.76	15.00
143	GLN	CA	-31.30	-13.45	50.40	15.00
143	GLN	CB	-30.10	-12.81	49.70	15.00
143	GLN	CG	-29.69	-11.45	50.28	15.00
143	GLN	CD	-28.34	-10.91	49.77	15.00
143	GLN	OE1	-27.73	-10.04	50.40	15.00
143	GLN	NE2	-27.85	-11.46	48.64	15.00
143	GLN	C	-32.50	-12.51	50.43	15.00
143	GLN	O	-32.76	-11.85	51.44	15.00
144	PHE	N	-33.28	-12.51	49.36	15.00
144	PHE	CA	-34.43	-11.62	49.26	15.00
144	PHE	CB	-34.43	-10.90	47.89	15.00

TABLE V

144 PHE CG	-33.21	-10.01	47.66	15.00
144 PHE CD1	-32.96	-8.92	48.48	15.00
144 PHE CD2	-32.31	-10.29	46.63	15.00
144 PHE CE1	-31.83	-8.12	48.30	15.00
144 PHE CE2	-31.17	-9.48	46.44	15.00
144 PHE CZ	-30.94	-8.40	47.27	15.00
144 PHE C	-35.79	-12.23	49.61	15.00
144 PHE O	-36.83	-11.62	49.35	15.00
145 TYR N	-35.78	-13.41	50.24	15.00
145 TYR CA	-37.03	-14.08	50.64	15.00
145 TYR CB	-36.76	-15.42	51.35	15.00
145 TYR CG	-37.96	-16.00	52.08	15.00
145 TYR CD1	-38.82	-16.92	51.46	15.00
145 TYR CE1	-39.93	-17.45	52.13	15.00
145 TYR CD2	-38.26	-15.62	53.38	15.00
145 TYR CE2	-39.37	-16.13	54.05	15.00
145 TYR CZ	-40.20	-17.04	53.43	15.00
145 TYR OH	-41.29	-17.54	54.12	15.00
145 TYR C	-37.90	-13.18	51.52	15.00
145 TYR O	-37.38	-12.43	52.36	15.00
146 SER N	-39.21	-13.31	51.38	15.00
146 SER CA	-40.13	-12.49	52.15	15.00
146 SER CB	-40.37	-11.15	51.45	15.00
146 SER OG	-40.91	-11.35	50.15	15.00
146 SER C	-41.46	-13.15	52.51	15.00
146 SER O	-41.95	-12.96	53.62	15.00
147 LYS N	-42.01	-13.92	51.58	15.00
147 LYS CA	-43.30	-14.59	51.76	15.00
147 LYS CB	-44.42	-13.76	51.10	15.00
147 LYS CG	-44.60	-12.34	51.62	15.00
147 LYS CD	-45.05	-12.34	53.08	15.00
147 LYS CE	-45.37	-10.92	53.58	15.00
147 LYS NZ	-46.00	-10.90	54.93	15.00
147 LYS C	-43.37	-16.03	51.20	15.00
147 LYS O	-42.63	-16.39	50.27	15.00
148 GLY N	-44.29	-16.81	51.75	15.00
148 GLY CA	-44.52	-18.16	51.28	15.00
148 GLY C	-43.46	-19.22	51.49	15.00
148 GLY O	-42.47	-18.99	52.18	15.00
149 VAL N	-43.70	-20.41	50.95	15.00
149 VAL CA	-42.78	-21.53	51.07	15.00
149 VAL CB	-43.53	-22.90	50.95	15.00

TABLE V

149 VAL CG1	-42.55	-24.07	50.90	15.00
149 VAL CG2	-44.47	-23.08	52.14	15.00
149 VAL C	-41.69	-21.41	50.01	15.00
149 VAL O	-41.94	-21.55	48.82	15.00
150 TYR N	-40.49	-21.08	50.48	15.00
150 TYR CA	-39.31	-20.92	49.63	15.00
150 TYR CB	-38.12	-20.36	50.42	15.00
150 TYR CG	-36.84	-20.29	49.60	15.00
150 TYR CD1	-36.67	-19.30	48.63	15.00
150 TYR CE1	-35.54	-19.29	47.81	15.00
150 TYR CD2	-35.84	-21.25	49.74	15.00
150 TYR CE2	-34.71	-21.24	48.92	15.00
150 TYR CZ	-34.57	-20.26	47.96	15.00
150 TYR OH	-33.48	-20.27	47.12	15.00
150 TYR C	-38.89	-22.18	48.89	15.00
150 TYR O	-38.88	-23.28	49.45	15.00
151 TYR N	-38.47	-21.98	47.65	15.00
151 TYR CA	-37.98	-23.03	46.77	15.00
151 TYR CB	-39.09	-23.99	46.35	15.00
151 TYR CG	-38.62	-25.09	45.42	15.00
151 TYR CD1	-37.92	-26.20	45.91	15.00
151 TYR CE1	-37.51	-27.23	45.06	15.00
151 TYR CD2	-38.89	-25.04	44.05	15.00
151 TYR CE2	-38.49	-26.07	43.19	15.00
151 TYR CZ	-37.80	-27.16	43.70	15.00
151 TYR OH	-37.46	-28.21	42.87	15.00
151 TYR C	-37.35	-22.39	45.55	15.00
151 TYR O	-37.80	-21.33	45.07	15.00
152 ASP N	-36.30	-23.02	45.05	15.00
152 ASP CA	-35.59	-22.54	43.86	15.00
152 ASP CB	-34.66	-21.38	44.20	15.00
152 ASP CG	-34.13	-20.68	42.97	15.00
152 ASP OD1	-33.52	-19.60	43.12	15.00
152 ASP OD2	-34.32	-21.20	41.84	15.00
152 ASP C	-34.83	-23.70	43.25	15.00
152 ASP O	-33.94	-24.27	43.89	15.00
153 GLU N	-35.15	-24.04	42.01	15.00
153 GLU CA	-34.50	-25.15	41.34	15.00
153 GLU CB	-35.16	-25.45	40.00	15.00
153 GLU CG	-34.95	-24.38	38.96	15.00
153 GLU CD	-35.39	-24.81	37.56	15.00
153 GLU OE1	-35.72	-26.00	37.37	15.00

TABLE V

153 GLU OE2	-35.40	-23.94	36.66	15.00
153 GLU C	-32.98	-25.02	41.17	15.00
153 GLU O	-32.30	-26.01	40.92	15.00
154 SER N	-32.46	-23.80	41.32	15.00
154 SER CA	-31.02	-23.56	41.18	15.00
154 SER CB	-30.77	-22.15	40.66	15.00
154 SER OG	-31.56	-21.91	39.50	15.00
154 SER C	-30.23	-23.82	42.46	15.00
154 SER O	-28.99	-23.76	42.45	15.00
155 CYS N	-30.94	-24.13	43.53	15.00
155 CYS CA	-30.35	-24.39	44.84	15.00
155 CYS C	-29.60	-25.71	44.92	15.00
155 CYS O	-30.20	-26.78	44.85	15.00
155 CYS CB	-31.43	-24.32	45.91	15.00
155 CYS SG	-30.84	-23.76	47.53	15.00
156 ASN N	-28.29	-25.64	45.11	15.00
156 ASN CA	-27.46	-26.84	45.20	15.00
156 ASN CB	-26.08	-26.58	44.61	15.00
156 ASN CG	-25.26	-27.85	44.48	15.00
156 ASN OD1	-25.77	-28.97	44.56	15.00
156 ASN ND2	-23.96	-27.69	44.26	15.00
156 ASN C	-27.33	-27.51	46.58	15.00
156 ASN O	-26.74	-26.95	47.51	15.00
157 SER N	-27.78	-28.76	46.65	15.00
157 SER CA	-27.73	-29.53	47.88	15.00
157 SER CB	-28.66	-30.74	47.80	15.00
157 SER OG	-28.22	-31.64	46.80	15.00
157 SER C	-26.33	-29.97	48.29	15.00
157 SER O	-26.16	-30.58	49.35	15.00
158 ASP N	-25.34	-29.71	47.43	15.00
158 ASP CA	-23.95	-30.07	47.71	15.00
158 ASP CB	-23.35	-30.92	46.59	15.00
158 ASP CG	-24.02	-32.27	46.47	15.00
158 ASP OD1	-24.01	-33.04	47.47	15.00
158 ASP OD2	-24.58	-32.55	45.38	15.00
158 ASP C	-23.09	-28.84	47.97	15.00
158 ASP O	-21.86	-28.90	47.96	15.00
159 ASN N	-23.76	-27.70	48.14	15.00
159 ASN CA	-23.08	-26.45	48.42	15.00
159 ASN CB	-23.32	-25.45	47.30	15.00
159 ASN CG	-22.57	-24.14	47.51	15.00
159 ASN OD1	-21.74	-24.00	48.41	15.00

TABLE V

159 ASN ND2	-22.86	-23.16	46.67	15.00
159 ASN C	-23.69	-25.99	49.73	15.00
159 ASN O	-24.50	-25.06	49.75	15.00
160 LEU N	-23.39	-26.71	50.81	15.00
160 LEU CA	-23.89	-26.38	52.15	15.00
160 LEU CB	-23.90	-27.62	53.06	15.00
160 LEU CG	-24.57	-28.92	52.58	15.00
160 LEU CD1	-24.38	-30.01	53.60	15.00
160 LEU CD2	-26.04	-28.72	52.33	15.00
160 LEU C	-23.01	-25.25	52.70	15.00
160 LEU O	-21.92	-25.48	53.22	15.00
161 ASN N	-23.52	-24.02	52.60	15.00
161 ASN CA	-22.76	-22.83	53.00	15.00
161 ASN CB	-22.57	-21.92	51.79	15.00
161 ASN CG	-23.88	-21.63	51.05	15.00
161 ASN OD1	-24.76	-20.95	51.55	15.00
161 ASN ND2	-24.00	-22.18	49.86	15.00
161 ASN C	-23.26	-22.01	54.20	15.00
161 ASN O	-22.55	-21.12	54.69	15.00
162 HIS N	-24.46	-22.32	54.68	15.00
162 HIS CA	-25.05	-21.57	55.79	15.00
162 HIS CB	-25.96	-20.49	55.23	15.00
162 HIS CG	-26.59	-19.59	56.25	15.00
162 HIS CD2	-27.87	-19.21	56.42	15.00
162 HIS ND1	-25.86	-18.91	57.21	15.00
162 HIS CE1	-26.66	-18.14	57.91	15.00
162 HIS NE2	-27.89	-18.30	57.45	15.00
162 HIS C	-25.78	-22.50	56.78	15.00
162 HIS O	-26.69	-23.22	56.39	15.00
163 ALA N	-25.32	-22.55	58.02	15.00
163 ALA CA	-25.96	-23.37	59.05	15.00
163 ALA CB	-24.98	-23.74	60.15	15.00
163 ALA C	-27.13	-22.57	59.62	15.00
163 ALA O	-26.96	-21.42	60.03	15.00
164 VAL N	-28.29	-23.20	59.71	15.00
164 VAL CA	-29.50	-22.54	60.16	15.00
164 VAL CB	-30.35	-22.26	58.88	15.00
164 VAL CG1	-31.36	-23.35	58.63	15.00
164 VAL CG2	-30.92	-20.89	58.89	15.00
164 VAL C	-30.20	-23.45	61.21	15.00
164 VAL O	-29.65	-24.48	61.57	15.00
165 LEU N	-31.35	-23.06	61.74	15.00

TABLE V

165 LEU CA	-32.05	-23.90	62.72	15.00
165 LEU CB	-32.05	-23.25	64.11	15.00
165 LEU CG	-32.78	-23.96	65.26	15.00
165 LEU CD1	-32.01	-25.18	65.72	15.00
165 LEU CD2	-32.97	-22.99	66.42	15.00
165 LEU C	-33.48	-24.25	62.31	15.00
165 LEU O	-34.26	-23.36	61.97	15.00
166 ALA N	-33.83	-25.54	62.36	15.00
166 ALA CA	-35.17	-26.00	62.00	15.00
166 ALA CB	-35.08	-27.37	61.33	15.00
166 ALA C	-36.09	-26.07	63.23	15.00
166 ALA O	-36.08	-27.05	63.97	15.00
167 VAL N	-36.92	-25.04	63.39	15.00
167 VAL CA	-37.82	-24.95	64.54	15.00
167 VAL CB	-37.90	-23.48	65.05	15.00
167 VAL CG1	-36.52	-22.98	65.43	15.00
167 VAL CG2	-38.52	-22.57	64.00	15.00
167 VAL C	-39.23	-25.53	64.35	15.00
167 VAL O	-40.12	-25.32	65.18	15.00
168 GLY N	-39.43	-26.27	63.27	15.00
168 GLY CA	-40.73	-26.86	63.04	15.00
168 GLY C	-40.94	-27.30	61.61	15.00
168 GLY O	-40.00	-27.42	60.82	15.00
169 TYR N	-42.21	-27.55	61.29	15.00
169 TYR CA	-42.63	-28.00	59.98	15.00
169 TYR CB	-42.14	-29.44	59.67	15.00
169 TYR CG	-42.65	-30.54	60.59	15.00
169 TYR CD1	-43.92	-31.12	60.41	15.00
169 TYR CE1	-44.37	-32.15	61.25	15.00
169 TYR CD2	-41.86	-31.02	61.63	15.00
169 TYR CE2	-42.31	-32.06	62.47	15.00
169 TYR CZ	-43.57	-32.61	62.27	15.00
169 TYR OH	-44.00	-33.61	63.11	15.00
169 TYR C	-44.14	-27.91	59.91	15.00
169 TYR O	-44.83	-27.98	60.92	15.00
170 GLY N	-44.65	-27.78	58.70	15.00
170 GLY CA	-46.08	-27.68	58.51	15.00
170 GLY C	-46.38	-27.73	57.04	15.00
170 GLY O	-45.57	-28.17	56.24	15.00
171 ILE N	-47.52	-27.17	56.68	15.00
171 ILE CA	-47.97	-27.14	55.30	15.00
171 ILE CB	-48.87	-28.38	55.01	15.00

TABLE V

171 ILE CG2	-49.85	-28.63	56.15	15.00
171 ILE CG1	-49.58	-28.25	53.67	15.00
171 ILE CD1	-50.27	-29.51	53.26	15.00
171 ILE C	-48.71	-25.83	55.06	15.00
171 ILE O	-49.51	-25.40	55.88	15.00
172 GLN N	-48.35	-25.13	53.99	15.00
172 GLN CA	-48.99	-23.87	53.65	15.00
172 GLN CB	-48.01	-22.70	53.72	15.00
172 GLN CG	-48.67	-21.36	53.62	15.00
172 GLN CD	-47.71	-20.23	53.89	15.00
172 GLN OE1	-47.35	-19.97	55.05	15.00
172 GLN NE2	-47.27	-19.55	52.84	15.00
172 GLN C	-49.60	-24.00	52.25	15.00
172 GLN O	-48.88	-24.13	51.26	15.00
173 LYS N	-50.93	-23.99	52.20	15.00
173 LYS CA	-51.68	-24.15	50.97	15.00
173 LYS CB	-51.66	-22.89	50.10	15.00
173 LYS CG	-52.38	-23.03	48.72	15.00
173 LYS CD	-53.92	-23.15	48.79	15.00
173 LYS CE	-54.45	-24.44	49.47	15.00
173 LYS NZ	-54.10	-25.73	48.79	15.00
173 LYS C	-51.15	-25.34	50.20	15.00
173 LYS O	-50.54	-25.19	49.14	15.00
174 GLY N	-51.31	-26.53	50.77	15.00
174 GLY CA	-50.84	-27.73	50.10	15.00
174 GLY C	-49.36	-27.74	49.76	15.00
174 GLY O	-48.95	-28.42	48.82	15.00
175 ASN N	-48.57	-26.97	50.50	15.00
175 ASN CA	-47.12	-26.90	50.30	15.00
175 ASN CB	-46.69	-25.54	49.74	15.00
175 ASN CG	-46.88	-25.43	48.24	15.00
175 ASN OD1	-45.91	-25.39	47.48	15.00
175 ASN ND2	-48.13	-25.38	47.79	15.00
175 ASN C	-46.40	-27.18	51.61	15.00
175 ASN O	-46.33	-26.31	52.49	15.00
176 LYS N	-45.91	-28.41	51.76	15.00
176 LYS CA	-45.18	-28.82	52.97	15.00
176 LYS CB	-44.88	-30.32	52.95	15.00
176 LYS CG	-46.14	-31.18	52.92	15.00
176 LYS CD	-45.83	-32.64	52.63	15.00
176 LYS CE	-47.08	-33.51	52.74	15.00
176 LYS NZ	-47.62	-33.57	54.13	15.00

TABLE V

176 LYS C	-43.90	-28.00	53.08	15.00
176 LYS O	-43.34	-27.58	52.07	15.00
177 HIS N	-43.42	-27.80	54.30	15.00
177 HIS CA	-42.23	-26.99	54.52	15.00
177 HIS CB	-42.58	-25.51	54.38	15.00
177 HIS CG	-43.53	-25.04	55.43	15.00
177 HIS CD2	-43.36	-24.83	56.76	15.00
177 HIS ND1	-44.87	-24.83	55.18	15.00
177 HIS CE1	-45.48	-24.50	56.31	15.00
177 HIS NE2	-44.59	-24.50	57.28	15.00
177 HIS C	-41.62	-27.24	55.88	15.00
177 HIS O	-42.21	-27.92	56.71	15.00
178 TRP N	-40.49	-26.58	56.12	15.00
178 TRP CA	-39.74	-26.60	57.38	15.00
178 TRP CB	-38.28	-27.02	57.18	15.00
178 TRP CG	-38.08	-28.36	56.62	15.00
178 TRP CD2	-38.10	-29.59	57.34	15.00
178 TRP CE2	-37.84	-30.62	56.41	15.00
178 TRP CE3	-38.30	-29.94	58.68	15.00
178 TRP CD1	-37.82	-28.67	55.32	15.00
178 TRP NE1	-37.68	-30.02	55.18	15.00
178 TRP CZ2	-37.79	-31.98	56.77	15.00
178 TRP CZ3	-38.25	-31.28	59.05	15.00
178 TRP CH2	-37.99	-32.28	58.09	15.00
178 TRP C	-39.76	-25.15	57.89	15.00
178 TRP O	-39.63	-24.21	57.10	15.00
179 ILE N	-39.96	-24.95	59.18	15.00
179 ILE CA	-39.96	-23.60	59.72	15.00
179 ILE CB	-40.92	-23.46	60.92	15.00
179 ILE CG2	-41.00	-22.01	61.38	15.00
179 ILE CG1	-42.33	-23.91	60.50	15.00
179 ILE CD1	-43.31	-23.94	61.64	15.00
179 ILE C	-38.50	-23.37	60.10	15.00
179 ILE O	-37.97	-24.03	61.00	15.00
180 ILE N	-37.84	-22.48	59.36	15.00
180 ILE CA	-36.43	-22.18	59.55	15.00
180 ILE CB	-35.67	-22.22	58.19	15.00
180 ILE CG2	-34.25	-21.74	58.35	15.00
180 ILE CG1	-35.73	-23.63	57.58	15.00
180 ILE CD1	-35.19	-24.73	58.48	15.00
180 ILE C	-36.14	-20.84	60.22	15.00
180 ILE O	-36.63	-19.80	59.79	15.00

TABLE V

181	LYS	N	-35.33	-20.88	61.27	15.00
181	LYS	CA	-34.93	-19.68	62.01	15.00
181	LYS	CB	-34.89	-19.94	63.51	15.00
181	LYS	CG	-34.35	-18.76	64.31	15.00
181	LYS	CD	-34.18	-19.11	65.77	15.00
181	LYS	CE	-33.68	-17.92	66.56	15.00
181	LYS	NZ	-33.51	-18.24	68.01	15.00
181	LYS	C	-33.55	-19.25	61.51	15.00
181	LYS	O	-32.61	-20.03	61.53	15.00
182	ASN	N	-33.43	-18.00	61.07	15.00
182	ASN	CA	-32.16	-17.49	60.56	15.00
182	ASN	CB	-32.35	-16.82	59.19	15.00
182	ASN	CG	-31.05	-16.69	58.41	15.00
182	ASN	OD1	-30.02	-17.26	58.78	15.00
182	ASN	ND2	-31.09	-15.95	57.31	15.00
182	ASN	C	-31.49	-16.53	61.56	15.00
182	ASN	O	-32.12	-16.09	62.52	15.00
183	SER	N	-30.20	-16.28	61.35	15.00
183	SER	CA	-29.44	-15.37	62.20	15.00
183	SER	CB	-28.30	-16.09	62.93	15.00
183	SER	OG	-27.53	-16.88	62.05	15.00
183	SER	C	-28.93	-14.14	61.42	15.00
183	SER	O	-27.77	-13.73	61.54	15.00
184	TRP	N	-29.81	-13.60	60.57	15.00
184	TRP	CA	-29.50	-12.41	59.78	15.00
184	TRP	CB	-29.71	-12.65	58.29	15.00
184	TRP	CG	-28.64	-13.47	57.67	15.00
184	TRP	CD2	-28.66	-14.06	56.37	15.00
184	TRP	CE2	-27.47	-14.81	56.23	15.00
184	TRP	CE3	-29.58	-14.04	55.31	15.00
184	TRP	CD1	-27.46	-13.86	58.25	15.00
184	TRP	NE1	-26.76	-14.67	57.39	15.00
184	TRP	CZ2	-27.18	-15.53	55.06	15.00
184	TRP	CZ3	-29.29	-14.76	54.16	15.00
184	TRP	CH2	-28.09	-15.49	54.04	15.00
184	TRP	C	-30.34	-11.22	60.27	15.00
184	TRP	O	-30.59	-10.27	59.53	15.00
185	GLY	N	-30.78	-11.31	61.52	15.00
185	GLY	CA	-31.57	-10.25	62.10	15.00
185	GLY	C	-33.05	-10.45	61.90	15.00
185	GLY	O	-33.50	-11.18	61.01	15.00
186	GLU	N	-33.81	-9.76	62.75	15.00

TABLE V

186 GLU CA	-35.27	-9.78	62.74	15.00
186 GLU CB	-35.81	-9.15	64.05	15.00
186 GLU CG	-37.34	-9.12	64.18	15.00
186 GLU CD	-37.84	-9.82	65.44	15.00
186 GLU OE1	-37.53	-9.33	66.55	15.00
186 GLU OE2	-38.54	-10.87	65.33	15.00
186 GLU C	-35.85	-9.11	61.50	15.00
186 GLU O	-36.99	-9.36	61.12	15.00
187 ASN N	-35.05	-8.27	60.84	15.00
187 ASN CA	-35.52	-7.59	59.64	15.00
187 ASN CB	-35.00	-6.16	59.56	15.00
187 ASN CG	-36.02	-5.17	60.07	15.00
187 ASN OD1	-35.91	-4.68	61.20	15.00
187 ASN ND2	-37.05	-4.90	59.25	15.00
187 ASN C	-35.23	-8.31	58.33	15.00
187 ASN O	-35.26	-7.72	57.27	15.00
188 TRP N	-34.94	-9.60	58.43	15.00
188 TRP CA	-34.68	-10.39	57.25	15.00
188 TRP CB	-33.32	-11.10	57.33	15.00
188 TRP CG	-33.12	-12.00	56.19	15.00
188 TRP CD2	-33.49	-13.38	56.12	15.00
188 TRP CE2	-33.22	-13.81	54.80	15.00
188 TRP CE3	-34.04	-14.29	57.03	15.00
188 TRP CD1	-32.64	-11.66	54.96	15.00
188 TRP NE1	-32.71	-12.74	54.12	15.00
188 TRP CZ2	-33.48	-15.13	54.37	15.00
188 TRP CZ3	-34.30	-15.60	56.60	15.00
188 TRP CH2	-34.02	-16.00	55.28	15.00
188 TRP C	-35.82	-11.39	57.10	15.00
188 TRP O	-36.41	-11.81	58.09	15.00
189 GLY N	-36.11	-11.76	55.85	15.00
189 GLY CA	-37.16	-12.72	55.57	15.00
189 GLY C	-38.43	-12.37	56.32	15.00
189 GLY O	-38.82	-11.20	56.40	15.00
190 ASN N	-39.08	-13.38	56.89	15.00
190 ASN CA	-40.30	-13.15	57.64	15.00
190 ASN CB	-41.37	-14.19	57.30	15.00
190 ASN CG	-42.78	-13.73	57.68	15.00
190 ASN OD1	-43.76	-14.38	57.34	15.00
190 ASN ND2	-42.88	-12.59	58.37	15.00
190 ASN C	-40.02	-13.14	59.13	15.00
190 ASN O	-40.22	-14.15	59.80	15.00

TABLE V

191 LYS N	-39.56	-11.99	59.63	15.00
191 LYS CA	-39.23	-11.78	61.05	15.00
191 LYS CB	-40.40	-12.11	61.99	15.00
191 LYS CG	-41.62	-11.23	61.84	15.00
191 LYS CD	-42.63	-11.52	62.95	15.00
191 LYS CE	-43.99	-10.85	62.71	15.00
191 LYS NZ	-44.94	-11.70	61.92	15.00
191 LYS C	-37.98	-12.58	61.45	15.00
191 LYS O	-37.79	-12.95	62.61	15.00
192 GLY N	-37.13	-12.82	60.45	15.00
192 GLY CA	-35.90	-13.56	60.66	15.00
192 GLY C	-36.13	-15.04	60.40	15.00
192 GLY O	-35.29	-15.88	60.72	15.00
193 TYR N	-37.28	-15.34	59.80	15.00
193 TYR CA	-37.66	-16.70	59.49	15.00
193 TYR CB	-38.91	-17.11	60.25	15.00
193 TYR CG	-38.66	-17.45	61.68	15.00
193 TYR CD1	-38.59	-16.46	62.66	15.00
193 TYR CE1	-38.33	-16.78	63.98	15.00
193 TYR CD2	-38.48	-18.78	62.07	15.00
193 TYR CE2	-38.22	-19.11	63.38	15.00
193 TYR CZ	-38.15	-18.11	64.34	15.00
193 TYR OH	-37.89	-18.43	65.64	15.00
193 TYR C	-37.86	-16.93	58.01	15.00
193 TYR O	-37.92	-15.99	57.22	15.00
194 ILE N	-37.97	-18.20	57.65	15.00
194 ILE CA	-38.20	-18.60	56.28	15.00
194 ILE CB	-36.88	-18.58	55.44	15.00
194 ILE CG2	-35.81	-19.44	56.08	15.00
194 ILE CG1	-37.16	-19.03	54.00	15.00
194 ILE CD1	-36.05	-18.68	53.02	15.00
194 ILE C	-38.85	-20.00	56.28	15.00
194 ILE O	-38.54	-20.83	57.14	15.00
195 LEU N	-39.84	-20.20	55.42	15.00
195 LEU CA	-40.50	-21.49	55.30	15.00
195 LEU CB	-42.00	-21.36	55.08	15.00
195 LEU CG	-42.81	-20.66	56.16	15.00
195 LEU CD1	-44.27	-20.65	55.77	15.00
195 LEU CD2	-42.60	-21.36	57.49	15.00
195 LEU C	-39.83	-22.09	54.09	15.00
195 LEU O	-39.85	-21.47	53.04	15.00
196 MET N	-39.17	-23.23	54.23	15.00

TABLE V

196 MET CA	-38.49	-23.84	53.10	15.00
196 MET CB	-37.01	-24.08	53.39	15.00
196 MET CG	-36.15	-22.83	53.37	15.00
196 MET SD	-34.45	-23.19	53.93	15.00
196 MET CE	-33.63	-23.67	52.36	15.00
196 MET C	-39.17	-25.14	52.72	15.00
196 MET O	-39.59	-25.89	53.59	15.00
197 ALA N	-39.22	-25.41	51.41	15.00
197 ALA CA	-39.86	-26.62	50.87	15.00
197 ALA CB	-39.64	-26.70	49.36	15.00
197 ALA C	-39.42	-27.93	51.53	15.00
197 ALA O	-38.23	-28.21	51.67	15.00
198 ARG N	-40.41	-28.73	51.91	15.00
198 ARG CA	-40.18	-30.01	52.57	15.00
198 ARG CB	-40.77	-30.03	53.98	15.00
198 ARG CG	-40.78	-31.39	54.66	15.00
198 ARG CD	-41.18	-31.28	56.12	15.00
198 ARG NE	-42.52	-30.73	56.31	15.00
198 ARG CZ	-43.63	-31.47	56.40	15.00
198 ARG NH1	-43.55	-32.80	56.31	15.00
198 ARG NH2	-44.80	-30.89	56.62	15.00
198 ARG C	-40.74	-31.13	51.71	15.00
198 ARG O	-41.84	-31.00	51.16	15.00
199 ASN N	-39.98	-32.21	51.61	15.00
199 ASN CA	-40.35	-33.37	50.81	15.00
199 ASN CB	-41.72	-33.92	51.23	15.00
199 ASN CG	-41.71	-34.55	52.61	15.00
199 ASN OD1	-40.67	-34.60	53.26	15.00
199 ASN ND2	-42.87	-35.01	53.07	15.00
199 ASN C	-40.31	-33.04	49.32	15.00
199 ASN O	-41.18	-33.43	48.57	15.00
200 LYS N	-39.30	-32.27	48.92	15.00
200 LYS CA	-39.13	-31.88	47.54	15.00
200 LYS CB	-39.46	-30.41	47.32	15.00
200 LYS CG	-39.74	-30.07	45.87	15.00
200 LYS CD	-41.24	-30.05	45.59	15.00
200 LYS CE	-41.92	-28.93	46.40	15.00
200 LYS NZ	-43.41	-28.84	46.21	15.00
200 LYS C	-37.68	-32.17	47.16	15.00
200 LYS O	-36.89	-31.26	46.91	15.00
201 ASN N	-37.34	-33.46	47.14	15.00
201 ASN CA	-36.00	-33.95	46.83	15.00

TABLE V

201 ASN CB	-35.78	-34.02	45.31	15.00
201 ASN CG	-36.19	-32.75	44.59	15.00
201 ASN OD1	-37.20	-32.72	43.87	15.00
201 ASN ND2	-35.40	-31.70	44.76	15.00
201 ASN C	-34.84	-33.24	47.54	15.00
201 ASN O	-33.84	-32.88	46.92	15.00
202 ASN N	-34.98	-33.11	48.86	15.00
202 ASN CA	-33.97	-32.49	49.74	15.00
202 ASN CB	-32.74	-33.42	49.89	15.00
202 ASN CG	-31.91	-33.12	51.13	15.00
202 ASN OD1	-32.36	-32.48	52.07	15.00
202 ASN ND2	-30.67	-33.60	51.13	15.00
202 ASN C	-33.56	-31.08	49.33	15.00
202 ASN O	-32.39	-30.82	49.02	15.00
203 ALA N	-34.51	-30.16	49.36	15.00
203 ALA H	-35.31	-30.45	49.85	15.00
203 ALA CA	-34.34	-28.77	48.93	15.00
203 ALA CB	-35.57	-27.93	49.27	15.00
203 ALA C	-33.15	-28.14	49.67	15.00
203 ALA O	-33.11	-27.98	50.89	15.00
204 CYS N	-32.16	-27.74	48.86	15.00
204 CYS CA	-30.95	-27.06	49.31	15.00
204 CYS C	-30.08	-27.85	50.28	15.00
204 CYS O	-29.25	-27.26	50.98	15.00
204 CYS CB	-31.27	-25.68	49.90	15.00
204 CYS SG	-32.21	-24.52	48.84	15.00
205 GLY N	-30.24	-29.17	50.32	15.00
205 GLY CA	-29.45	-29.99	51.22	15.00
205 GLY C	-29.93	-29.89	52.66	15.00
205 GLY O	-29.14	-30.07	53.60	15.00
206 ILE N	-31.23	-29.68	52.83	15.00
206 ILE CA	-31.84	-29.52	54.15	15.00
206 ILE CB	-33.39	-29.24	54.01	15.00
206 ILE CG2	-34.12	-30.44	53.42	15.00
206 ILE CG1	-34.00	-28.84	55.35	15.00
206 ILE CD1	-33.66	-27.44	55.81	15.00
206 ILE C	-31.57	-30.69	55.11	15.00
206 ILE O	-31.39	-30.47	56.31	15.00
207 ALA N	-31.46	-31.91	54.59	15.00
207 ALA CA	-31.21	-33.09	55.42	15.00
207 ALA CB	-32.32	-34.12	55.21	15.00
207 ALA C	-29.83	-33.73	55.24	15.00

TABLE V

207 ALA O	-29.58	-34.86	55.66	15.00
208 ASN N	-28.92	-32.98	54.65	15.00
208 ASN CA	-27.58	-33.50	54.42	15.00
208 ASN CB	-26.91	-32.79	53.25	15.00
208 ASN CG	-27.23	-33.43	51.92	15.00
208 ASN OD1	-27.61	-34.59	51.86	15.00
208 ASN ND2	-27.06	-32.67	50.84	15.00
208 ASN C	-26.68	-33.44	55.65	15.00
208 ASN O	-25.80	-34.29	55.81	15.00
209 LEU N	-26.91	-32.46	56.52	15.00
209 LEU CA	-26.09	-32.29	57.72	15.00
209 LEU CB	-24.96	-31.30	57.44	15.00
209 LEU CG	-23.70	-31.44	58.30	15.00
209 LEU CD1	-22.81	-32.53	57.75	15.00
209 LEU CD2	-22.95	-30.12	58.33	15.00
209 LEU C	-26.86	-31.91	58.99	15.00
209 LEU O	-26.42	-31.04	59.74	15.00
210 ALA N	-27.99	-32.56	59.23	15.00
210 ALA H	-27.89	-32.43	58.64	15.00
210 ALA CA	-28.78	-32.25	60.42	15.00
210 ALA CB	-29.43	-31.67	60.51	15.00
210 ALA C	-28.24	-33.03	61.63	15.00
210 ALA O	-27.87	-34.20	61.51	15.00
211 SER N	-28.17	-32.35	62.78	15.00
211 SER CA	-27.71	-32.98	64.03	15.00
211 SER CB	-26.19	-33.01	64.15	15.00
211 SER OG	-25.65	-31.71	64.29	15.00
211 SER C	-28.32	-32.28	65.24	15.00
211 SER O	-28.93	-31.20	65.11	15.00
212 PHE N	-28.18	-32.89	66.41	15.00
212 PHE CA	-28.74	-32.30	67.61	15.00
212 PHE CB	-30.25	-32.56	67.71	15.00
212 PHE CG	-30.62	-34.00	67.79	15.00
212 PHE CD1	-31.04	-34.69	66.66	15.00
212 PHE CD2	-30.53	-34.69	69.00	15.00
212 PHE CE1	-31.36	-36.03	66.73	15.00
212 PHE CE2	-30.85	-36.04	69.07	15.00
212 PHE CZ	-31.27	-36.71	67.94	15.00
212 PHE C	-28.01	-32.78	68.87	15.00
212 PHE O	-27.55	-33.94	68.95	15.00
213 PRO N	-27.92	-31.91	69.88	15.00
213 PRO CD	-28.60	-30.60	69.99	15.00

TABLE V

213	PRO CA	-27.25	-32.25	71.13	15.00
213	PRO CB	-27.11	-30.89	71.80	15.00
213	PRO CG	-28.44	-30.26	71.47	15.00
213	PRO C	-28.13	-33.17	71.96	15.00
213	PRO O	-29.36	-33.23	71.79	15.00
214	LYS N	-27.48	-33.94	72.82	15.00
214	LYS CA	-28.19	-34.82	73.72	15.00
214	LYS CB	-27.71	-36.27	73.59	15.00
214	LYS CG	-27.91	-36.90	72.23	15.00
214	LYS CD	-27.28	-38.29	72.16	15.00
214	LYS CE	-25.79	-38.27	72.50	15.00
214	LYS NZ	-25.11	-39.56	72.18	15.00
214	LYS C	-27.84	-34.26	75.07	15.00
214	LYS O	-26.76	-33.71	75.24	15.00
215	MET N	-28.79	-34.27	75.99	15.00
215	MET CA	-28.55	-33.78	77.34	15.00
215	MET CB	-29.47	-32.60	77.70	15.00
215	MET CG	-29.12	-31.30	76.96	15.00
215	MET SD	-29.59	-29.73	77.80	15.00
215	MET CE	-28.68	-28.54	76.81	15.00
215	MET C	-28.66	-34.93	78.34	15.00
215	MET OT1	-27.81	-35.01	79.26	15.00
215	MET OT2	-29.54	-35.80	78.16	15.00
216	HOH OH2	-40.32	-20.86	90.40	15.00
217	HOH OH2	-20.71	-32.43	79.67	15.00
218	HOH OH2	-31.33	-16.38	65.47	15.00
219	HOH OH2	-29.76	-17.63	70.42	15.00
220	HOH OH2	-7.13	-18.39	66.48	15.00
221	HOH OH2	-15.45	-12.55	73.01	15.00
222	HOH OH2	-34.69	-23.23	69.94	15.00
223	HOH OH2	-11.03	-30.64	72.74	15.00
224	HOH OH2	-30.92	-18.33	68.20	15.00
225	HOH OH2	-24.49	-30.79	61.59	15.00
226	HOH OH2	-15.06	-10.95	61.61	15.00
227	HOH OH2	-14.14	-21.84	66.38	15.00
228	HOH OH2	-45.46	-29.94	49.49	15.00
229	HOH OH2	-45.53	-34.98	55.75	15.00
230	HOH OH2	-37.47	-12.36	67.54	15.00
231	HOH OH2	-32.59	-13.97	60.21	15.00
232	HOH OH2	-23.45	-33.51	51.76	15.00
233	HOH OH2	-9.95	-25.41	63.34	15.00
234	HOH OH2	-57.83	-31.91	39.28	15.00

TABLE V

235	HOH	OH2	-30.05	-20.10	63.45	15.00
236	HOH	OH2	-22.11	-29.91	61.97	15.00
237	HOH	OH2	-26.54	-11.16	68.27	15.00
238	HOH	OH2	-28.19	-16.14	71.94	15.00
239	HOH	OH2	-26.07	-26.03	83.66	15.00
240	HOH	OH2	-35.84	-27.16	51.26	15.00
241	HOH	OH2	-35.66	-24.80	49.57	15.00
242	HOH	OH2	-46.96	-32.65	56.91	15.00
243	HOH	OH2	-25.39	-9.00	77.82	15.00
244	HOH	OH2	-41.61	-14.85	64.38	15.00
245	HOH	OH2	-18.39	-3.01	63.15	15.00
246	HOH	OH2	-33.49	-28.51	70.47	15.00
247	HOH	OH2	-48.24	-19.58	79.27	15.00
248	HOH	OH2	-17.16	-11.08	74.86	15.00
249	HOH	OH2	-7.77	-18.99	72.85	15.00
250	HOH	OH2	-12.50	-24.63	81.88	15.00
251	HOH	OH2	-28.11	-35.31	58.10	15.00
252	HOH	OH2	-35.24	-11.03	53.39	15.00
253	HOH	OH2	-31.85	-28.95	46.18	15.00
254	HOH	OH2	-35.11	-24.97	46.75	15.00
255	HOH	OH2	-42.46	-38.44	54.37	15.00
256	HOH	OH2	-37.82	-16.40	67.58	15.00
257	HOH	OH2	-43.11	-16.23	66.45	15.00
258	HOH	OH2	-36.79	-9.70	73.69	15.00
259	HOH	OH2	-34.92	-15.40	75.95	15.00
260	HOH	OH2	-32.03	-7.39	60.30	15.00
261	HOH	OH2	-19.94	-8.07	62.81	15.00
262	HOH	OH2	-33.79	-20.76	69.68	15.00
263	HOH	OH2	-33.86	-45.02	74.42	15.00
264	HOH	OH2	-11.97	-27.02	71.08	15.00
265	HOH	OH2	-8.26	-25.33	61.28	15.00
266	HOH	OH2	-19.53	-42.28	58.81	15.00
267	HOH	OH2	-20.68	-32.75	61.19	15.00
268	HOH	OH2	-24.87	-33.89	60.62	15.00
269	HOH	OH2	-2.83	-32.79	71.85	15.00
270	HOH	OH2	-14.43	-40.52	59.53	15.00
271	HOH	OH2	-21.46	-37.41	78.35	15.00
272	HOH	OH2	-19.79	-36.03	71.33	15.00
273	HOH	OH2	-28.57	-35.40	88.70	15.00
274	HOH	OH2	-13.04	-12.02	63.26	15.00
275	HOH	OH2	-8.63	-11.89	72.80	15.00
276	HOH	OH2	-28.58	-30.13	56.41	15.00

TABLE V

277	HOH	OH2	-29.86	-20.69	48.27	15.00
278	HOH	OH2	-26.77	-22.94	44.37	15.00
279	HOH	OH2	-25.17	-36.24	49.68	15.00
280	HOH	OH2	-19.40	-31.57	49.99	15.00
281	HOH	OH2	-34.95	-29.42	45.52	15.00
282	HOH	OH2	-37.69	-30.43	50.51	15.00

TABLE VI

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for the cathepsin K complex with inhibitor 2-[N-(3-benzyloxybenzoyl)]-2'-[N'-(N-benzyloxycarbonyl-L-leuciny)]carbohydrazide.

Residue Atom	X	Y	Z	B
1 ALA CB	-53.28	-28.69	64.46	15.00
1 ALA C	-53.74	-30.77	63.13	15.00
1 ALA O	-54.17	-31.71	63.79	15.00
1 ALA N	-55.61	-29.36	63.92	15.00
1 ALA CA	-54.20	-29.34	63.43	15.00
2 PRO N	-52.92	-30.93	62.07	15.00
2 PRO CD	-52.55	-29.87	61.11	15.00
2 PRO CA	-52.38	-32.23	61.65	15.00
2 PRO CB	-52.22	-32.03	60.15	15.00
2 PRO CG	-51.68	-30.61	60.09	15.00
2 PRO C	-51.02	-32.37	62.31	15.00
2 PRO O	-50.88	-32.09	63.50	15.00
3 ASP N	-50.02	-32.75	61.52	15.00
3 ASP CA	-48.67	-32.92	62.02	15.00
3 ASP CB	-47.96	-34.03	61.25	15.00
3 ASP CG	-48.48	-35.41	61.59	15.00
3 ASP OD1	-49.68	-35.69	61.38	15.00
3 ASP OD2	-47.66	-36.24	62.06	15.00
3 ASP C	-47.93	-31.60	61.84	15.00
3 ASP O	-47.35	-31.34	60.78	15.00
4 SER N	-48.02	-30.74	62.84	15.00
4 SER CA	-47.34	-29.45	62.82	15.00
4 SER CB	-48.32	-28.34	62.42	15.00
4 SER OG	-48.91	-28.65	61.17	15.00
4 SER C	-46.76	-29.17	64.20	15.00
4 SER O	-47.33	-29.58	65.22	15.00
5 VAL N	-45.60	-28.54	64.23	15.00
5 VAL CA	-45.00	-28.20	65.51	15.00
5 VAL CB	-44.16	-29.36	66.11	15.00
5 VAL CG1	-42.89	-29.57	65.35	15.00
5 VAL CG2	-43.87	-29.08	67.57	15.00
5 VAL C	-44.21	-26.91	65.37	15.00
5 VAL O	-43.46	-26.73	64.41	15.00
6 ASP N	-44.48	-25.98	66.27	15.00

TABLE III

108 ARG CD	-26.86	-36.86	79.28	15.00
108 ARG NE	-26.63	-38.14	78.60	15.00
108 ARG CZ	-27.58	-38.89	78.03	15.00
108 ARG NH1	-28.85	-38.51	78.05	15.00
108 ARG NH2	-27.24	-40.03	77.45	15.00
108 ARG C	-23.64	-35.78	76.18	15.00
108 ARG O	-23.84	-36.99	76.06	15.00
109 GLY N	-23.20	-35.03	75.17	15.00
109 GLY CA	-22.97	-35.63	73.87	15.00
109 GLY C	-23.82	-34.99	72.80	15.00
109 GLY O	-24.27	-33.85	72.95	15.00
110 TYR N	-24.09	-35.72	71.72	15.00
110 TYR CA	-24.89	-35.19	70.63	15.00
110 TYR CB	-24.12	-34.08	69.91	15.00
110 TYR CG	-22.86	-34.56	69.20	15.00
110 TYR CD1	-21.64	-34.62	69.87	15.00
110 TYR CE1	-20.49	-35.03	69.22	15.00
110 TYR CD2	-22.90	-34.93	67.85	15.00
110 TYR CE2	-21.75	-35.34	67.19	15.00
110 TYR CZ	-20.55	-35.39	67.88	15.00
110 TYR OH	-19.39	-35.77	67.23	15.00
110 TYR C	-25.22	-36.28	69.62	15.00
110 TYR O	-24.44	-37.21	69.43	15.00
111 ARG N	-26.34	-36.11	68.92	15.00
111 ARG CA	-26.76	-37.08	67.92	15.00
111 ARG CB	-28.02	-37.81	68.38	15.00
111 ARG CG	-27.81	-38.84	69.48	15.00
111 ARG CD	-28.75	-40.03	69.33	15.00
111 ARG NE	-28.01	-41.28	69.36	15.00
111 ARG CZ	-27.89	-42.06	70.44	15.00
111 ARG NH1	-27.18	-43.18	70.36	15.00
111 ARG NH2	-28.50	-41.73	71.58	15.00
111 ARG C	-26.99	-36.46	66.54	15.00
111 ARG O	-27.67	-35.45	66.41	15.00
112 GLU N	-26.41	-37.06	65.50	15.00
112 GLU CA	-26.56	-36.57	64.14	15.00
112 GLU CB	-25.36	-37.00	63.29	15.00
112 GLU CG	-24.03	-36.42	63.76	15.00
112 GLU CD	-23.34	-35.56	62.70	15.00
112 GLU OE1	-23.95	-34.57	62.22	15.00
112 GLU OE2	-22.18	-35.88	62.33	15.00
112 GLU C	-27.86	-37.13	63.56	15.00
112 GLU O	-28.64	-37.75	64.27	15.00

TABLE III

113 ILE N	-28.13	-36.87	62.29	15.00
113 ILE CA	-29.35	-37.38	61.64	15.00
113 ILE CB	-30.38	-36.25	61.34	15.00
113 ILE CG2	-31.67	-36.83	60.78	15.00
113 ILE CG1	-30.71	-35.45	62.60	15.00
113 ILE CD1	-31.50	-36.20	63.65	15.00
113 ILE C	-28.85	-37.98	60.33	15.00
113 ILE O	-27.91	-37.46	59.73	15.00
114 PRO N	-29.41	-39.13	59.92	15.00
114 PRO CD	-30.48	-39.91	60.57	15.00
114 PRO CA	-28.98	-39.77	58.68	15.00
114 PRO CB	-30.10	-40.78	58.43	15.00
114 PRO CG	-30.41	-41.23	59.83	15.00
114 PRO C	-28.87	-38.79	57.54	15.00
114 PRO O	-29.84	-38.12	57.20	15.00
115 GLU N	-27.67	-38.66	56.99	15.00
115 GLU CA	-27.46	-37.74	55.89	15.00
115 GLU CB	-26.07	-37.92	55.28	15.00
115 GLU CG	-24.92	-37.19	56.01	15.00
115 GLU CD	-23.60	-37.16	55.20	15.00
115 GLU OE1	-23.65	-37.20	53.94	15.00
115 GLU OE2	-22.51	-37.08	55.82	15.00
115 GLU C	-28.53	-37.91	54.82	15.00
115 GLU O	-28.70	-39.00	54.27	15.00
116 GLY N	-29.27	-36.83	54.59	15.00
116 GLY CA	-30.30	-36.78	53.57	15.00
116 GLY C	-31.63	-37.36	53.99	15.00
116 GLY O	-32.46	-37.66	53.13	15.00
117 ASN N	-31.88	-37.44	55.29	15.00
117 ASN CA	-33.12	-38.03	55.77	15.00
117 ASN CB	-32.80	-39.09	56.82	15.00
117 ASN CG	-33.80	-40.21	56.84	15.00
117 ASN OD1	-35.02	-39.99	56.90	15.00
117 ASN ND2	-33.31	-41.44	56.76	15.00
117 ASN C	-34.17	-37.06	56.31	15.00
117 ASN O	-34.17	-36.72	57.50	15.00
118 GLU N	-35.12	-36.66	55.48	15.00
118 GLU CA	-36.15	-35.72	55.91	15.00
118 GLU CB	-36.86	-35.08	54.72	15.00
118 GLU CG	-36.09	-33.98	54.02	15.00
118 GLU CD	-36.99	-33.14	53.15	15.00
118 GLU OE1	-36.58	-32.75	52.04	15.00
118 GLU OE2	-38.13	-32.87	53.57	15.00

TABLE III

118	GLU C	-37.18	-36.33	56.83	15.00
118	GLU O	-37.76	-35.64	57.66	15.00
119	LYS N	-37.46	-37.61	56.66	15.00
119	LYS CA	-38.43	-38.29	57.53	15.00
119	LYS CB	-38.66	-39.71	57.03	15.00
119	LYS CG	-39.20	-39.77	55.60	15.00
119	LYS CD	-40.54	-39.04	55.49	15.00
119	LYS CE	-41.04	-38.97	54.07	15.00
119	LYS NZ	-40.26	-38.00	53.26	15.00
119	LYS C	-37.89	-38.30	58.95	15.00
119	LYS O	-38.55	-37.86	59.89	15.00
120	ALA N	-36.64	-38.74	59.07	15.00
120	ALA CA	-35.94	-38.81	60.34	15.00
120	ALA CB	-34.58	-39.42	60.15	15.00
120	ALA C	-35.81	-37.43	60.97	15.00
120	ALA O	-35.88	-37.28	62.19	15.00
121	LEU N	-35.56	-36.42	60.14	15.00
121	LEU CA	-35.43	-35.06	60.66	15.00
121	LEU CB	-34.96	-34.10	59.56	15.00
121	LEU CG	-34.93	-32.61	59.96	15.00
121	LEU CD1	-33.81	-32.34	60.93	15.00
121	LEU CD2	-34.78	-31.76	58.72	15.00
121	LEU C	-36.76	-34.60	61.25	15.00
121	LEU O	-36.81	-33.98	62.31	15.00
122	LYS N	-37.86	-34.91	60.57	15.00
122	LYS CA	-39.17	-34.53	61.06	15.00
122	LYS CB	-40.26	-35.04	60.11	15.00
122	LYS CG	-41.65	-34.70	60.59	15.00
122	LYS CD	-42.73	-35.28	59.72	15.00
122	LYS CE	-44.10	-34.79	60.19	15.00
122	LYS NZ	-45.21	-35.17	59.28	15.00
122	LYS C	-39.36	-35.15	62.43	15.00
122	LYS O	-39.79	-34.47	63.36	15.00
123	ARG N	-39.02	-36.44	62.55	15.00
123	ARG CA	-39.13	-37.17	63.81	15.00
123	ARG CB	-38.72	-38.64	63.64	15.00
123	ARG CG	-39.86	-39.56	63.26	15.00
123	ARG CD	-39.43	-41.02	63.33	15.00
123	ARG NE	-38.71	-41.48	62.14	15.00
123	ARG CZ	-37.42	-41.79	62.12	15.00
123	ARG NH1	-36.68	-41.70	63.21	15.00
123	ARG NH2	-36.87	-42.22	60.99	15.00
123	ARG C	-38.28	-36.55	64.90	15.00

TABLE III

123 ARG O	-38.69	-36.51	66.05	15.00
124 ALA N	-37.09	-36.07	64.55	15.00
124 ALA CA	-36.20	-35.45	65.52	15.00
124 ALA CB	-34.85	-35.18	64.89	15.00
124 ALA C	-36.81	-34.15	66.03	15.00
124 ALA O	-36.96	-33.96	67.23	15.00
125 VAL N	-37.17	-33.25	65.12	15.00
125 VAL CA	-37.77	-31.97	65.50	15.00
125 VAL CB	-38.07	-31.11	64.25	15.00
125 VAL CG1	-38.97	-29.94	64.59	15.00
125 VAL CG2	-36.78	-30.59	63.67	15.00
125 VAL C	-39.04	-32.20	66.30	15.00
125 VAL O	-39.36	-31.43	67.20	15.00
126 ALA N	-39.74	-33.29	66.00	15.00
126 ALA CA	-40.97	-33.62	66.69	15.00
126 ALA CB	-41.78	-34.61	65.88	15.00
126 ALA C	-40.72	-34.17	68.09	15.00
126 ALA O	-41.37	-33.76	69.06	15.00
127 ARG N	-39.77	-35.10	68.19	15.00
127 ARG CA	-39.41	-35.74	69.44	15.00
127 ARG CB	-38.71	-37.07	69.18	15.00
127 ARG CG	-39.58	-38.30	69.27	15.00
127 ARG CD	-40.17	-38.70	67.94	15.00
127 ARG NE	-39.87	-40.09	67.60	15.00
127 ARG CZ	-40.52	-40.78	66.67	15.00
127 ARG NH1	-40.18	-42.03	66.40	15.00
127 ARG NH2	-41.55	-40.25	66.03	15.00
127 ARG C	-38.52	-34.91	70.35	15.00
127 ARG O	-38.86	-34.71	71.52	15.00
128 VAL N	-37.37	-34.50	69.82	15.00
128 VAL CA	-36.36	-33.72	70.56	15.00
128 VAL CB	-34.95	-33.91	69.94	15.00
128 VAL CG1	-33.88	-33.45	70.91	15.00
128 VAL CG2	-34.73	-35.35	69.57	15.00
128 VAL C	-36.62	-32.22	70.66	15.00
128 VAL O	-36.44	-31.61	71.71	15.00
129 GLY N	-36.99	-31.60	69.55	15.00
129 GLY CA	-37.23	-30.17	69.54	15.00
129 GLY C	-36.29	-29.54	68.53	15.00
129 GLY O	-35.87	-30.22	67.58	15.00
130 PRO N	-35.94	-28.25	68.71	15.00
130 PRO CD	-36.46	-27.38	69.78	15.00
130 PRO CA	-35.04	-27.50	67.83	15.00

TABLE III

130 PRO CB	-34.80	-26.22	68.62	15.00
130 PRO CG	-36.12	-26.00	69.26	15.00
130 PRO C	-33.74	-28.21	67.50	15.00
130 PRO O	-32.90	-28.46	68.37	15.00
131 VAL N	-33.59	-28.51	66.21	15.00
131 VAL CA	-32.42	-29.19	65.68	15.00
131 VAL CB	-32.84	-30.34	64.73	15.00
131 VAL CG1	-31.64	-31.06	64.18	15.00
131 VAL CG2	-33.74	-31.33	65.48	15.00
131 VAL C	-31.57	-28.19	64.90	15.00
131 VAL O	-32.08	-27.25	64.28	15.00
132 SER N	-30.25	-28.38	64.96	15.00
132 SER CA	-29.32	-27.53	64.26	15.00
132 SER CB	-28.00	-27.48	65.02	15.00
132 SER OG	-28.18	-26.93	66.31	15.00
132 SER C	-29.08	-28.14	62.88	15.00
132 SER O	-28.67	-29.30	62.79	15.00
133 VAL N	-29.38	-27.38	61.83	15.00
133 VAL CA	-29.21	-27.83	60.44	15.00
133 VAL CB	-30.57	-27.93	59.68	15.00
133 VAL CG1	-31.55	-28.81	60.43	15.00
133 VAL CG2	-31.16	-26.56	59.49	15.00
133 VAL C	-28.30	-26.86	59.68	15.00
133 VAL O	-28.06	-25.74	60.13	15.00
134 ALA N	-27.79	-27.28	58.52	15.00
134 ALA CA	-26.94	-26.44	57.69	15.00
134 ALA CB	-25.50	-26.93	57.73	15.00
134 ALA C	-27.49	-26.50	56.28	15.00
134 ALA O	-27.84	-27.57	55.79	15.00
135 ILE N	-27.58	-25.36	55.61	15.00
135 ILE CA	-28.14	-25.32	54.27	15.00
135 ILE CB	-29.58	-24.73	54.30	15.00
135 ILE CG2	-30.49	-25.57	55.19	15.00
135 ILE CG1	-29.53	-23.26	54.76	15.00
135 ILE CD1	-30.88	-22.58	54.88	15.00
135 ILE C	-27.33	-24.44	53.32	15.00
135 ILE O	-26.33	-23.82	53.72	15.00
136 ASP N	-27.75	-24.41	52.05	15.00
136 ASP CA	-27.12	-23.57	51.05	15.00
136 ASP CB	-27.25	-24.16	49.65	15.00
136 ASP CG	-26.77	-23.20	48.57	15.00
136 ASP OD1	-27.27	-23.28	47.43	15.00
136 ASP OD2	-25.90	-22.35	48.85	15.00

TABLE III

136 ASP C	-27.87	-22.24	51.10	15.00
136 ASP O	-29.05	-22.17	50.77	15.00
137 ALA N	-27.19	-21.21	51.59	15.00
137 ALA CA	-27.80	-19.89	51.68	15.00
137 ALA CB	-27.61	-19.32	53.08	15.00
137 ALA C	-27.23	-18.94	50.62	15.00
137 ALA O	-27.64	-17.78	50.53	15.00
138 SER N	-26.26	-19.43	49.84	15.00
138 SER CA	-25.66	-18.65	48.77	15.00
138 SER CB	-24.30	-19.22	48.37	15.00
138 SER OG	-23.28	-18.86	49.30	15.00
138 SER C	-26.61	-18.73	47.60	15.00
138 SER O	-26.51	-19.65	46.80	15.00
139 LEU N	-27.54	-17.77	47.57	15.00
139 LEU CA	-28.59	-17.66	46.55	15.00
139 LEU CB	-29.53	-18.86	46.65	15.00
139 LEU CG	-29.89	-19.63	45.38	15.00
139 LEU CD1	-28.66	-20.27	44.80	15.00
139 LEU CD2	-30.92	-20.68	45.71	15.00
139 LEU C	-29.39	-16.39	46.85	15.00
139 LEU O	-29.91	-16.22	47.96	15.00
140 THR N	-29.52	-15.49	45.87	15.00
140 THR CA	-30.23	-14.23	46.08	15.00
140 THR CB	-30.06	-13.28	44.87	15.00
140 THR OG1	-29.05	-13.81	43.99	15.00
140 THR CG2	-29.62	-11.89	45.34	15.00
140 THR C	-31.71	-14.37	46.42	15.00
140 THR O	-32.23	-13.63	47.24	15.00
141 SER N	-32.39	-15.35	45.83	15.00
141 SER CA	-33.80	-15.59	46.10	15.00
141 SER CB	-34.31	-16.76	45.27	15.00
141 SER OG	-33.42	-17.86	45.34	15.00
141 SER C	-34.00	-15.89	47.57	15.00
141 SER O	-35.03	-15.57	48.16	15.00
142 PHE N	-33.01	-16.51	48.18	15.00
142 PHE CA	-33.07	-16.86	49.59	15.00
142 PHE CB	-31.98	-17.88	49.93	15.00
142 PHE CG	-31.93	-18.24	51.39	15.00
142 PHE CD1	-32.72	-19.25	51.89	15.00
142 PHE CD2	-31.10	-17.54	52.25	15.00
142 PHE CE1	-32.68	-19.58	53.23	15.00
142 PHE CE2	-31.05	-17.85	53.60	15.00
142 PHE CZ	-31.85	-18.87	54.09	15.00

TABLE III

142	PHE C	-32.88	-15.61	50.43	15.00
142	PHE O	-33.66	-15.33	51.34	15.00
143	GLN N	-31.86	-14.84	50.09	15.00
143	GLN CA	-31.54	-13.64	50.83	15.00
143	GLN CB	-30.25	-13.06	50.30	15.00
143	GLN CG	-29.18	-14.11	50.24	15.00
143	GLN CD	-27.84	-13.53	49.97	15.00
143	GLN OE1	-27.41	-12.58	50.62	15.00
143	GLN NE2	-27.15	-14.10	48.99	15.00
143	GLN C	-32.63	-12.59	50.89	15.00
143	GLN O	-32.90	-12.05	51.95	15.00
144	PHE N	-33.29	-12.29	49.77	15.00
144	PHE CA	-34.36	-11.28	49.80	15.00
144	PHE CB	-34.33	-10.38	48.55	15.00
144	PHE CG	-34.46	-11.12	47.24	15.00
144	PHE CD1	-33.45	-11.04	46.30	15.00
144	PHE CD2	-35.59	-11.87	46.95	15.00
144	PHE CE1	-33.56	-11.71	45.09	15.00
144	PHE CE2	-35.71	-12.55	45.75	15.00
144	PHE CZ	-34.70	-12.46	44.82	15.00
144	PHE C	-35.76	-11.83	50.04	15.00
144	PHE O	-36.76	-11.19	49.68	15.00
145	TYR N	-35.83	-13.01	50.66	15.00
145	TYR CA	-37.09	-13.68	50.97	15.00
145	TYR CB	-36.80	-15.04	51.62	15.00
145	TYR CG	-37.95	-15.65	52.36	15.00
145	TYR CD1	-38.83	-16.52	51.73	15.00
145	TYR CE1	-39.93	-17.05	52.41	15.00
145	TYR CD2	-38.20	-15.31	53.69	15.00
145	TYR CE2	-39.28	-15.83	54.38	15.00
145	TYR CZ	-40.14	-16.69	53.73	15.00
145	TYR OH	-41.24	-17.16	54.42	15.00
145	TYR C	-37.87	-12.81	51.93	15.00
145	TYR O	-37.27	-12.10	52.74	15.00
146	SER N	-39.20	-12.88	51.89	15.00
146	SER CA	-40.01	-12.07	52.78	15.00
146	SER CB	-40.45	-10.78	52.10	15.00
146	SER OG	-41.31	-11.05	51.01	15.00
146	SER C	-41.23	-12.81	53.34	15.00
146	SER O	-41.69	-12.52	54.45	15.00
147	LYS N	-41.77	-13.75	52.58	15.00
147	LYS CA	-42.93	-14.52	53.04	15.00
147	LYS CB	-44.16	-13.62	53.21	15.00

TABLE III

147 LYS CG	-44.84	-13.14	51.92	15.00
147 LYS CD	-45.64	-11.86	52.19	15.00
147 LYS CE	-44.71	-10.72	52.70	15.00
147 LYS NZ	-45.41	-9.52	53.28	15.00
147 LYS C	-43.27	-15.68	52.11	15.00
147 LYS O	-43.03	-15.62	50.91	15.00
148 GLY N	-43.83	-16.74	52.69	15.00
148 GLY CA	-44.21	-17.90	51.90	15.00
148 GLY C	-43.31	-19.08	52.16	15.00
148 GLY O	-42.50	-19.07	53.08	15.00
149 VAL N	-43.46	-20.12	51.35	15.00
149 VAL CA	-42.65	-21.32	51.50	15.00
149 VAL CB	-43.52	-22.60	51.39	15.00
149 VAL CG1	-42.66	-23.84	51.53	15.00
149 VAL CG2	-44.59	-22.59	52.45	15.00
149 VAL C	-41.57	-21.27	50.42	15.00
149 VAL O	-41.84	-21.44	49.24	15.00
150 TYR N	-40.34	-21.01	50.84	15.00
150 TYR CA	-39.21	-20.90	49.93	15.00
150 TYR CB	-37.98	-20.37	50.67	15.00
150 TYR CG	-36.75	-20.27	49.80	15.00
150 TYR CD1	-36.73	-19.44	48.68	15.00
150 TYR CE1	-35.61	-19.36	47.86	15.00
150 TYR CD2	-35.61	-21.03	50.09	15.00
150 TYR CE2	-34.48	-20.96	49.27	15.00
150 TYR CZ	-34.49	-20.13	48.16	15.00
150 TYR OH	-33.41	-20.06	47.32	15.00
150 TYR C	-38.81	-22.16	49.19	15.00
150 TYR O	-38.56	-23.19	49.80	15.00
151 TYR N	-38.68	-22.03	47.88	15.00
151 TYR CA	-38.24	-23.13	47.02	15.00
151 TYR CB	-39.38	-24.11	46.72	15.00
151 TYR CG	-38.89	-25.32	45.96	15.00
151 TYR CD1	-37.74	-26.01	46.37	15.00
151 TYR CE1	-37.23	-27.06	45.63	15.00
151 TYR CD2	-39.52	-25.74	44.79	15.00
151 TYR CE2	-39.01	-26.80	44.03	15.00
151 TYR CZ	-37.87	-27.45	44.46	15.00
151 TYR OH	-37.35	-28.50	43.72	15.00
151 TYR C	-37.63	-22.58	45.73	15.00
151 TYR O	-38.19	-21.69	45.08	15.00
152 ASP N	-36.47	-23.12	45.37	15.00
152 ASP CA	-35.74	-22.69	44.19	15.00

TABLE III

152 ASP CB	-34.80	-21.56	44.59	15.00
152 ASP CG	-34.09	-20.92	43.42	15.00
152 ASP OD1	-33.27	-21.60	42.76	15.00
152 ASP OD2	-34.35	-19.73	43.17	15.00
152 ASP C	-34.93	-23.88	43.70	15.00
152 ASP O	-33.98	-24.30	44.37	15.00
153 GLU N	-35.23	-24.36	42.51	15.00
153 GLU CA	-34.55	-25.53	41.95	15.00
153 GLU CB	-35.15	-25.91	40.59	15.00
153 GLU CG	-35.40	-24.74	39.62	15.00
153 GLU CD	-34.12	-24.02	39.16	15.00
153 GLU OE1	-33.16	-24.68	38.70	15.00
153 GLU OE2	-34.09	-22.76	39.27	15.00
153 GLU C	-33.03	-25.50	41.88	15.00
153 GLU O	-32.40	-26.49	41.49	15.00
154 SER N	-32.42	-24.37	42.22	15.00
154 SER CA	-30.96	-24.26	42.18	15.00
154 SER CB	-30.53	-23.00	41.43	15.00
154 SER OG	-30.93	-23.09	40.06	15.00
154 SER C	-30.27	-24.34	43.55	15.00
154 SER O	-29.04	-24.33	43.65	15.00
155 CYS N	-31.06	-24.43	44.61	15.00
155 CYS CA	-30.49	-24.54	45.95	15.00
155 CYS C	-29.66	-25.81	45.88	15.00
155 CYS O	-30.16	-26.88	45.54	15.00
155 CYS CB	-31.60	-24.69	46.96	15.00
155 CYS SG	-31.20	-23.89	48.53	15.00
156 ASN N	-28.36	-25.70	46.16	15.00
156 ASN CA	-27.50	-26.87	46.05	15.00
156 ASN CB	-26.20	-26.49	45.36	15.00
156 ASN CG	-25.34	-27.69	45.04	15.00
156 ASN OD1	-25.83	-28.82	44.97	15.00
156 ASN ND2	-24.05	-27.47	44.88	15.00
156 ASN C	-27.21	-27.66	47.33	15.00
156 ASN O	-26.37	-27.26	48.13	15.00
157 SER N	-27.82	-28.83	47.43	15.00
157 SER CA	-27.66	-29.72	48.57	15.00
157 SER CB	-28.41	-31.03	48.33	15.00
157 SER OG	-29.78	-30.78	48.03	15.00
157 SER C	-26.19	-30.04	48.87	15.00
157 SER O	-25.86	-30.54	49.96	15.00
158 ASP N	-25.31	-29.75	47.92	15.00
158 ASP CA	-23.89	-30.03	48.07	15.00

TABLE III

158 ASP CB	-23.30	-30.43	46.71	15.00
158 ASP CG	-24.01	-31.63	46.08	15.00
158 ASP OD1	-25.23	-31.53	45.79	15.00
158 ASP OD2	-23.34	-32.67	45.86	15.00
158 ASP C	-23.11	-28.86	48.64	15.00
158 ASP O	-22.00	-29.02	49.15	15.00
159 ASN N	-23.68	-27.66	48.60	15.00
159 ASN CA	-22.98	-26.49	49.11	15.00
159 ASN CB	-23.02	-25.36	48.07	15.00
159 ASN CG	-21.95	-24.29	48.31	15.00
159 ASN OD1	-21.61	-23.96	49.45	15.00
159 ASN ND2	-21.43	-23.72	47.22	15.00
159 ASN C	-23.59	-26.01	50.41	15.00
159 ASN O	-24.34	-25.03	50.44	15.00
160 LEU N	-23.31	-26.69	51.52	15.00
160 LEU CA	-23.86	-26.27	52.80	15.00
160 LEU CB	-23.99	-27.45	53.77	15.00
160 LEU CG	-24.87	-28.62	53.30	15.00
160 LEU CD1	-25.08	-29.56	54.47	15.00
160 LEU CD2	-26.21	-28.16	52.76	15.00
160 LEU C	-22.91	-25.21	53.33	15.00
160 LEU O	-21.77	-25.51	53.65	15.00
161 ASN N	-23.38	-23.97	53.35	15.00
161 ASN CA	-22.55	-22.84	53.78	15.00
161 ASN CB	-22.32	-21.90	52.60	15.00
161 ASN CG	-23.61	-21.59	51.84	15.00
161 ASN OD1	-24.49	-20.86	52.31	15.00
161 ASN ND2	-23.75	-22.18	50.66	15.00
161 ASN C	-23.10	-22.04	54.94	15.00
161 ASN O	-22.37	-21.29	55.58	15.00
162 HIS N	-24.38	-22.20	55.24	15.00
162 HIS CA	-25.01	-21.44	56.31	15.00
162 HIS CB	-26.00	-20.43	55.72	15.00
162 HIS CG	-26.46	-19.38	56.68	15.00
162 HIS CD2	-27.69	-18.91	56.97	15.00
162 HIS ND1	-25.58	-18.66	57.46	15.00
162 HIS CE1	-26.25	-17.79	58.19	15.00
162 HIS NE2	-27.54	-17.92	57.90	15.00
162 HIS C	-25.74	-22.34	57.31	15.00
162 HIS O	-26.66	-23.07	56.94	15.00
163 ALA N	-25.31	-22.30	58.57	15.00
163 ALA CA	-25.93	-23.09	59.63	15.00
163 ALA CB	-24.98	-23.25	60.81	15.00

TABLE III

163 ALA C	-27.18	-22.33	60.08	15.00
163 ALA O	-27.20	-21.09	60.08	15.00
164 VAL N	-28.21	-23.05	60.48	15.00
164 VAL CA	-29.44	-22.43	60.91	15.00
164 VAL CB	-30.31	-22.10	59.66	15.00
164 VAL CG1	-31.25	-23.23	59.31	15.00
164 VAL CG2	-30.99	-20.79	59.85	15.00
164 VAL C	-30.13	-23.35	61.91	15.00
164 VAL O	-29.51	-24.32	62.35	15.00
165 LEU N	-31.38	-23.10	62.28	15.00
165 LEU CA	-32.05	-23.93	63.28	15.00
165 LEU CB	-31.95	-23.25	64.64	15.00
165 LEU CG	-32.41	-23.97	65.90	15.00
165 LEU CD1	-31.39	-25.01	66.31	15.00
165 LEU CD2	-32.58	-22.96	67.00	15.00
165 LEU C	-33.51	-24.20	62.98	15.00
165 LEU O	-34.30	-23.27	62.86	15.00
166 ALA N	-33.88	-25.48	62.93	15.00
166 ALA CA	-35.27	-25.89	62.66	15.00
166 ALA CB	-35.30	-27.31	62.15	15.00
166 ALA C	-36.07	-25.78	63.95	15.00
166 ALA O	-35.74	-26.40	64.95	15.00
167 VAL N	-37.14	-24.99	63.93	15.00
167 VAL CA	-38.00	-24.75	65.09	15.00
167 VAL CB	-38.22	-23.21	65.30	15.00
167 VAL CG1	-39.07	-22.93	66.50	15.00
167 VAL CG2	-36.88	-22.50	65.47	15.00
167 VAL C	-39.35	-25.46	64.93	15.00
167 VAL O	-40.25	-25.34	65.77	15.00
168 GLY N	-39.51	-26.21	63.85	15.00
168 GLY CA	-40.75	-26.91	63.61	15.00
168 GLY C	-40.97	-27.18	62.14	15.00
168 GLY O	-40.03	-27.15	61.35	15.00
169 TYR N	-42.22	-27.45	61.78	15.00
169 TYR CA	-42.63	-27.75	60.41	15.00
169 TYR CB	-42.23	-29.18	60.00	15.00
169 TYR CG	-42.72	-30.27	60.93	15.00
169 TYR CD1	-44.07	-30.66	60.94	15.00
169 TYR CE1	-44.52	-31.66	61.81	15.00
169 TYR CD2	-41.85	-30.91	61.81	15.00
169 TYR CE2	-42.29	-31.91	62.68	15.00
169 TYR CZ	-43.63	-32.27	62.68	15.00
169 TYR OH	-44.07	-33.24	63.57	15.00

TABLE III

169 TYR C	-44.14	-27.59	60.31	15.00
169 TYR O	-44.81	-27.32	61.30	15.00
170 GLY N	-44.70	-27.76	59.12	15.00
170 GLY CA	-46.14	-27.63	58.97	15.00
170 GLY C	-46.56	-27.53	57.52	15.00
170 GLY O	-45.85	-27.94	56.61	15.00
171 ILE N	-47.74	-26.97	57.30	15.00
171 ILE CA	-48.28	-26.78	55.97	15.00
171 ILE CB	-49.43	-27.78	55.69	15.00
171 ILE CG2	-50.14	-27.44	54.38	15.00
171 ILE CG1	-48.91	-29.22	55.69	15.00
171 ILE CD1	-48.38	-29.69	54.35	15.00
171 ILE C	-48.89	-25.40	56.05	15.00
171 ILE O	-49.85	-25.20	56.78	15.00
172 GLN N	-48.29	-24.41	55.40	15.00
172 GLN CA	-48.86	-23.07	55.47	15.00
172 GLN CB	-47.96	-22.05	54.75	15.00
172 GLN CG	-48.37	-20.59	54.97	15.00
172 GLN CD	-47.48	-19.62	54.20	15.00
172 GLN OE1	-46.94	-19.96	53.14	15.00
172 GLN NE2	-47.33	-18.41	54.72	15.00
172 GLN C	-50.22	-23.15	54.78	15.00
172 GLN O	-51.26	-22.82	55.37	15.00
173 LYS N	-50.21	-23.61	53.54	15.00
173 LYS CA	-51.45	-23.77	52.79	15.00
173 LYS CB	-52.00	-22.41	52.33	15.00
173 LYS CG	-53.53	-22.35	52.25	15.00
173 LYS CD	-54.00	-20.89	52.22	15.00
173 LYS CE	-55.51	-20.75	52.34	15.00
173 LYS NZ	-55.91	-19.31	52.33	15.00
173 LYS C	-51.07	-24.63	51.61	15.00
173 LYS O	-50.50	-24.16	50.63	15.00
174 GLY N	-51.28	-25.93	51.80	15.00
174 GLY CA	-50.97	-26.89	50.76	15.00
174 GLY C	-49.51	-27.27	50.74	15.00
174 GLY O	-49.17	-28.42	50.45	15.00
175 ASN N	-48.63	-26.34	51.08	15.00
175 ASN CA	-47.20	-26.64	51.05	15.00
175 ASN CB	-46.44	-25.52	50.34	15.00
175 ASN CG	-46.88	-25.35	48.88	15.00
175 ASN OD1	-47.59	-24.39	48.54	15.00
175 ASN ND2	-46.49	-26.29	48.03	15.00
175 ASN C	-46.52	-26.98	52.38	15.00

TABLE III

175 ASN O	-46.58	-26.21	53.35	15.00
176 LYS N	-45.88	-28.15	52.40	15.00
176 LYS CA	-45.15	-28.65	53.56	15.00
176 LYS CB	-44.68	-30.09	53.34	15.00
176 LYS CG	-45.74	-31.03	52.77	15.00
176 LYS CD	-45.35	-32.49	52.97	15.00
176 LYS CE	-46.23	-33.44	52.14	15.00
176 LYS NZ	-45.80	-33.48	50.70	15.00
176 LYS C	-43.94	-27.75	53.75	15.00
176 LYS O	-43.26	-27.41	52.78	15.00
177 HIS N	-43.64	-27.39	55.00	15.00
177 HIS CA	-42.51	-26.50	55.25	15.00
177 HIS CB	-42.96	-25.05	55.09	15.00
177 HIS CG	-43.85	-24.56	56.20	15.00
177 HIS CD2	-43.59	-24.27	57.49	15.00
177 HIS ND1	-45.16	-24.20	55.99	15.00
177 HIS CE1	-45.67	-23.71	57.10	15.00
177 HIS NE2	-44.74	-23.75	58.03	15.00
177 HIS C	-41.82	-26.66	56.59	15.00
177 HIS O	-42.44	-27.05	57.57	15.00
178 TRP N	-40.52	-26.34	56.60	15.00
178 TRP CA	-39.67	-26.38	57.77	15.00
178 TRP CB	-38.26	-26.80	57.38	15.00
178 TRP CG	-38.11	-28.21	56.93	15.00
178 TRP CD2	-38.28	-29.38	57.73	15.00
178 TRP CE2	-38.02	-30.49	56.90	15.00
178 TRP CE3	-38.62	-29.60	59.08	15.00
178 TRP CD1	-37.77	-28.64	55.68	15.00
178 TRP NE1	-37.71	-30.01	55.65	15.00
178 TRP CZ2	-38.09	-31.80	57.37	15.00
178 TRP CZ3	-38.69	-30.89	59.54	15.00
178 TRP CH2	-38.43	-31.98	58.68	15.00
178 TRP C	-39.59	-24.94	58.28	15.00
178 TRP O	-39.26	-24.03	57.51	15.00
179 ILE N	-39.92	-24.71	59.55	15.00
179 ILE CA	-39.85	-23.36	60.09	15.00
179 ILE CB	-40.86	-23.17	61.23	15.00
179 ILE CG2	-40.80	-21.75	61.74	15.00
179 ILE CG1	-42.27	-23.50	60.72	15.00
179 ILE CD1	-43.38	-23.28	61.70	15.00
179 ILE C	-38.42	-23.13	60.55	15.00
179 ILE O	-37.94	-23.79	61.47	15.00
180 ILE N	-37.73	-22.22	59.88	15.00

TABLE III

180 ILE CA	-36.32	-21.94	60.17	15.00
180 ILE CB	-35.50	-22.02	58.86	15.00
180 ILE CG2	-34.06	-21.71	59.13	15.00
180 ILE CG1	-35.63	-23.40	58.22	15.00
180 ILE CD1	-34.94	-24.48	58.99	15.00
180 ILE C	-36.01	-20.62	60.88	15.00
180 ILE O	-36.59	-19.58	60.56	15.00
181 LYS N	-35.09	-20.68	61.84	15.00
181 LYS CA	-34.67	-19.51	62.60	15.00
181 LYS CB	-34.58	-19.83	64.09	15.00
181 LYS CG	-34.19	-18.62	64.93	15.00
181 LYS CD	-33.86	-18.95	66.37	15.00
181 LYS CE	-33.68	-17.66	67.16	15.00
181 LYS NZ	-33.07	-17.85	68.50	15.00
181 LYS C	-33.30	-19.10	62.12	15.00
181 LYS O	-32.31	-19.74	62.48	15.00
182 ASN N	-33.22	-18.04	61.32	15.00
182 ASN CA	-31.93	-17.56	60.79	15.00
182 ASN CB	-32.17	-16.80	59.48	15.00
182 ASN CG	-30.98	-16.86	58.53	15.00
182 ASN OD1	-29.87	-17.20	58.92	15.00
182 ASN ND2	-31.21	-16.50	57.27	15.00
182 ASN C	-31.29	-16.65	61.84	15.00
182 ASN O	-31.86	-16.44	62.91	15.00
183 SER N	-30.11	-16.11	61.56	15.00
183 SER CA	-29.44	-15.21	62.52	15.00
183 SER CB	-28.26	-15.93	63.18	15.00
183 SER CG	-27.41	-16.54	62.21	15.00
183 SER C	-28.98	-13.90	61.87	15.00
183 SER O	-27.84	-13.44	62.08	15.00
184 TRP N	-29.85	-13.26	61.11	15.00
184 TRP CA	-29.52	-12.01	60.45	15.00
184 TRP CB	-29.70	-12.14	58.94	15.00
184 TRP CG	-28.74	-13.05	58.26	15.00
184 TRP CD2	-28.89	-13.61	56.96	15.00
184 TRP CE2	-27.72	-14.38	56.71	15.00
184 TRP CE3	-29.87	-13.53	55.98	15.00
184 TRP CD1	-27.54	-13.48	58.74	15.00
184 TRP NE1	-26.92	-14.29	57.81	15.00
184 TRP CZ2	-27.53	-15.07	55.51	15.00
184 TRP CZ3	-29.68	-14.22	54.78	15.00
184 TRP CH2	-28.52	-14.98	54.56	15.00
184 TRP C	-30.45	-10.91	60.98	15.00

TABLE III

184 TRP O	-31.16	-10.28	60.20	15.00
185 GLY N	-30.48	-10.71	62.29	15.00
185 GLY CA	-31.34	-9.69	62.86	15.00
185 GLY C	-32.79	-10.02	62.61	15.00
185 GLY O	-33.09	-11.01	61.96	15.00
186 GLU N	-33.73	-9.25	63.14	15.00
186 GLU CA	-35.13	-9.57	62.89	15.00
186 GLU CB	-36.01	-9.41	64.14	15.00
186 GLU CG	-36.02	-8.04	64.75	15.00
186 GLU CD	-37.04	-7.92	65.87	15.00
186 GLU OE1	-36.66	-7.55	67.00	15.00
186 GLU OE2	-38.23	-8.21	65.61	15.00
186 GLU C	-35.67	-8.78	61.72	15.00
186 GLU O	-36.84	-8.91	61.34	15.00
187 ASN N	-34.80	-7.96	61.13	15.00
187 ASN CA	-35.17	-7.15	59.99	15.00
187 ASN CB	-34.20	-5.97	59.84	15.00
187 ASN CG	-34.83	-4.76	59.13	15.00
187 ASN OD1	-34.15	-4.03	58.42	15.00
187 ASN ND2	-36.12	-4.54	59.36	15.00
187 ASN C	-35.15	-8.03	58.74	15.00
187 ASN O	-35.75	-7.72	57.72	15.00
188 TRP N	-34.45	-9.16	58.81	15.00
188 TRP CA	-34.37	-10.07	57.66	15.00
188 TRP CB	-33.13	-10.97	57.77	15.00
188 TRP CG	-33.03	-11.92	56.63	15.00
188 TRP CD2	-33.46	-13.29	56.62	15.00
188 TRP CE2	-33.26	-13.77	55.31	15.00
188 TRP CE3	-34.00	-14.15	57.58	15.00
188 TRP CD1	-32.60	-11.64	55.38	15.00
188 TRP NE1	-32.73	-12.74	54.58	15.00
188 TRP CZ2	-33.58	-15.08	54.93	15.00
188 TRP CZ3	-34.31	-15.45	57.20	15.00
188 TRP CH2	-34.10	-15.90	55.89	15.00
188 TRP C	-35.63	-10.94	57.55	15.00
188 TRP O	-36.34	-11.13	58.54	15.00
189 GLY N	-35.89	-11.44	56.34	15.00
189 GLY CA	-37.04	-12.29	56.09	15.00
189 GLY C	-38.26	-11.99	56.92	15.00
189 GLY O	-38.56	-10.84	57.23	15.00
190 ASN N	-38.99	-13.02	57.32	15.00
190 ASN CA	-40.18	-12.81	58.14	15.00
190 ASN CB	-41.17	-13.96	57.97	15.00

TABLE III

190 ASN CG	-42.58	-13.57	58.36	15.00
190 ASN OD1	-43.53	-13.95	57.69	15.00
190 ASN ND2	-42.72	-12.80	59.43	15.00
190 ASN C	-39.79	-12.68	59.61	15.00
190 ASN O	-39.86	-13.65	60.36	15.00
191 LYS N	-39.41	-11.47	60.02	15.00
191 LYS CA	-39.01	-11.18	61.41	15.00
191 LYS CB	-40.23	-11.26	62.34	15.00
191 LYS CG	-41.41	-10.38	61.96	15.00
191 LYS CD	-42.64	-10.75	62.79	15.00
191 LYS CE	-43.93	-10.18	62.20	15.00
191 LYS NZ	-45.15	-10.69	62.91	15.00
191 LYS C	-37.94	-12.14	61.90	15.00
191 LYS O	-38.00	-12.62	63.03	15.00
192 GLY N	-36.97	-12.45	61.05	15.00
192 GLY CA	-35.91	-13.35	61.43	15.00
192 GLY C	-36.06	-14.79	60.97	15.00
192 GLY O	-35.07	-15.51	60.83	15.00
193 TYR N	-37.30	-15.21	60.70	15.00
193 TYR CA	-37.56	-16.59	60.27	15.00
193 TYR CB	-38.79	-17.14	61.01	15.00
193 TYR CG	-38.57	-17.28	62.49	15.00
193 TYR CD1	-38.77	-16.20	63.35	15.00
193 TYR CE1	-38.49	-16.30	64.70	15.00
193 TYR CD2	-38.09	-18.47	63.04	15.00
193 TYR CE2	-37.81	-18.58	64.40	15.00
193 TYR CZ	-38.00	-17.48	65.22	15.00
193 TYR OH	-37.69	-17.57	66.55	15.00
193 TYR C	-37.77	-16.76	58.76	15.00
193 TYR O	-37.85	-15.80	57.99	15.00
194 ILE N	-37.83	-18.01	58.33	15.00
194 ILE CA	-38.06	-18.34	56.94	15.00
194 ILE CB	-36.77	-18.17	56.07	15.00
194 ILE CG2	-35.64	-19.02	56.60	15.00
194 ILE CG1	-37.07	-18.54	54.62	15.00
194 ILE CD1	-35.87	-18.54	53.71	15.00
194 ILE C	-38.59	-19.77	56.84	15.00
194 ILE O	-38.12	-20.68	57.53	15.00
195 LEU N	-39.65	-19.93	56.06	15.00
195 LEU CA	-40.27	-21.23	55.84	15.00
195 LEU CB	-41.76	-21.08	55.61	15.00
195 LEU CG	-42.62	-21.03	56.88	15.00
195 LEU CD1	-41.90	-20.32	58.01	15.00

TABLE III

195 LEU CD2	-43.94	-20.37	56.58	15.00
195 LEU C	-39.61	-21.79	54.60	15.00
195 LEU O	-39.53	-21.13	53.57	15.00
196 MET N	-39.08	-23.00	54.71	15.00
196 MET CA	-38.42	-23.63	53.58	15.00
196 MET CB	-36.96	-23.90	53.93	15.00
196 MET CG	-36.13	-22.63	54.11	15.00
196 MET SD	-34.43	-22.96	54.57	15.00
196 MET CE	-33.85	-23.77	53.09	15.00
196 MET C	-39.17	-24.90	53.20	15.00
196 MET O	-39.74	-25.58	54.05	15.00
197 ALA N	-39.23	-25.22	51.91	15.00
197 ALA CA	-39.93	-26.41	51.45	15.00
197 ALA CB	-39.79	-26.55	49.94	15.00
197 ALA C	-39.51	-27.70	52.15	15.00
197 ALA O	-38.32	-27.92	52.41	15.00
198 ARG N	-40.50	-28.53	52.47	15.00
198 ARG CA	-40.29	-29.81	53.12	15.00
198 ARG CB	-40.95	-29.84	54.50	15.00
198 ARG CG	-40.91	-31.22	55.15	15.00
198 ARG CD	-41.22	-31.19	56.63	15.00
198 ARG NE	-42.59	-30.84	56.98	15.00
198 ARG CZ	-43.60	-31.70	56.98	15.00
198 ARG NH1	-43.40	-32.96	56.63	15.00
198 ARG NH2	-44.79	-31.32	57.43	15.00
198 ARG C	-40.86	-30.94	52.27	15.00
198 ARG O	-42.03	-30.91	51.88	15.00
199 ASN N	-40.00	-31.90	51.96	15.00
199 ASN CA	-40.33	-33.08	51.17	15.00
199 ASN CB	-41.68	-33.69	51.58	15.00
199 ASN CG	-41.66	-34.26	53.00	15.00
199 ASN OD1	-42.63	-34.12	53.74	15.00
199 ASN ND2	-40.55	-34.91	53.38	15.00
199 ASN C	-40.22	-32.89	49.66	15.00
199 ASN O	-40.46	-33.83	48.89	15.00
200 LYS N	-39.80	-31.71	49.23	15.00
200 LYS CA	-39.60	-31.45	47.81	15.00
200 LYS CB	-39.83	-29.98	47.45	15.00
200 LYS CG	-41.27	-29.52	47.67	15.00
200 LYS CD	-41.61	-28.27	46.88	15.00
200 LYS CE	-43.08	-27.86	47.07	15.00
200 LYS NZ	-43.51	-26.73	46.16	15.00
200 LYS C	-38.15	-31.86	47.56	15.00

TABLE III

200 LYS O	-37.29	-31.02	47.31	15.00
201 ASN N	-37.90	-33.15	47.74	15.00
201 ASN CA	-36.58	-33.74	47.55	15.00
201 ASN CB	-36.23	-33.86	46.06	15.00
201 ASN CG	-37.27	-34.62	45.25	15.00
201 ASN OD1	-37.46	-34.34	44.06	15.00
201 ASN ND2	-37.96	-35.58	45.88	15.00
201 ASN C	-35.48	-32.95	48.24	15.00
201 ASN O	-34.88	-32.07	47.64	15.00
202 ASN N	-35.27	-33.23	49.53	15.00
202 ASN CA	-34.21	-32.62	50.34	15.00
202 ASN CB	-33.01	-33.56	50.33	15.00
202 ASN CG	-31.96	-33.20	51.34	15.00
202 ASN OD1	-32.27	-32.76	52.45	15.00
202 ASN ND2	-30.71	-33.41	50.98	15.00
202 ASN C	-33.81	-31.18	49.94	15.00
202 ASN O	-32.63	-30.88	49.70	15.00
203 ALA N	-34.78	-30.29	49.91	15.00
203 ALA H	-35.58	-30.58	50.39	15.00
203 ALA CA	-34.60	-28.89	49.49	15.00
203 ALA CB	-35.83	-28.06	49.83	15.00
203 ALA C	-33.41	-28.27	50.25	15.00
203 ALA O	-33.31	-28.25	51.47	15.00
204 CYS N	-32.47	-27.71	49.46	15.00
204 CYS CA	-31.31	-27.02	50.02	15.00
204 CYS C	-30.43	-27.87	50.92	15.00
204 CYS O	-29.53	-27.34	51.59	15.00
204 CYS CB	-31.78	-25.79	50.79	15.00
204 CYS SG	-32.67	-24.58	49.75	15.00
205 GLY N	-30.64	-29.19	50.92	15.00
205 GLY CA	-29.86	-30.06	51.76	15.00
205 GLY C	-30.07	-29.75	53.23	15.00
205 GLY O	-29.14	-29.81	54.04	15.00
206 ILE N	-31.29	-29.37	53.59	15.00
206 ILE CA	-31.60	-29.06	54.98	15.00
206 ILE CB	-33.08	-28.64	55.16	15.00
206 ILE CG2	-34.01	-29.71	54.60	15.00
206 ILE CG1	-33.38	-28.40	56.63	15.00
206 ILE CD1	-34.65	-27.65	56.89	15.00
206 ILE C	-31.30	-30.24	55.91	15.00
206 ILE O	-30.92	-30.05	57.07	15.00
207 ALA N	-31.42	-31.46	55.39	15.00
207 ALA CA	-31.16	-32.64	56.19	15.00

TABLE III

207 ALA CB	-32.30	-33.64	56.03	15.00
207 ALA C	-29.82	-33.31	55.92	15.00
207 ALA O	-29.71	-34.52	55.99	15.00
208 ASN N	-28.75	-32.54	55.69	15.00
208 ASN CA	-27.44	-33.14	55.41	15.00
208 ASN CB	-26.91	-32.66	54.07	15.00
208 ASN CG	-27.50	-33.42	52.92	15.00
208 ASN OD1	-28.69	-33.32	52.66	15.00
208 ASN ND2	-26.68	-34.22	52.24	15.00
208 ASN C	-26.38	-32.91	56.46	15.00
208 ASN O	-25.30	-33.49	56.40	15.00
209 LEU N	-26.65	-32.01	57.40	15.00
209 LEU CA	-25.71	-31.72	58.47	15.00
209 LEU CB	-24.78	-30.58	58.07	15.00
209 LEU CG	-23.44	-30.57	58.80	15.00
209 LEU CD1	-22.65	-31.81	58.41	15.00
209 LEU CD2	-22.65	-29.33	58.46	15.00
209 LEU C	-26.52	-31.34	59.69	15.00
209 LEU O	-26.24	-30.34	60.34	15.00
210 ALA N	-27.55	-32.13	59.94	15.00
210 ALA H	-27.87	-32.61	59.15	15.00
210 ALA CA	-28.41	-31.91	61.10	15.00
210 ALA CB	-29.82	-32.45	60.85	15.00
210 ALA C	-27.84	-32.66	62.31	15.00
210 ALA O	-27.12	-33.64	62.12	15.00
211 SER N	-28.10	-32.14	63.49	15.00
211 SER CA	-27.62	-32.76	64.72	15.00
211 SER CB	-26.11	-32.53	64.90	15.00
211 SER OG	-25.80	-31.16	65.02	15.00
211 SER C	-28.35	-32.12	65.88	15.00
211 SER O	-28.97	-31.08	65.73	15.00
212 PHE N	-28.31	-32.77	67.03	15.00
212 PHE CA	-28.95	-32.21	68.21	15.00
212 PHE CB	-30.43	-32.63	68.32	15.00
212 PHE CG	-30.66	-34.13	68.43	15.00
212 PHE CD1	-31.05	-34.86	67.32	15.00
212 PHE CD2	-30.55	-34.79	69.67	15.00
212 PHE CE1	-31.34	-36.23	67.44	15.00
212 PHE CE2	-30.83	-36.15	69.79	15.00
212 PHE CZ	-31.23	-36.86	68.67	15.00
212 PHE C	-28.14	-32.62	69.42	15.00
212 PHE O	-27.50	-33.67	69.42	15.00
213 PRO N	-28.02	-31.73	70.40	15.00

TABLE III

213 PRO CD	-28.49	-30.34	70.46	15.00
213 PRO CA	-27.25	-32.08	71.59	15.00
213 PRO CB	-26.99	-30.73	72.23	15.00
213 PRO CG	-28.24	-29.98	71.91	15.00
213 PRO C	-28.08	-32.96	72.51	15.00
213 PRO O	-29.31	-32.92	72.48	15.00
214 LYS N	-27.43	-33.79	73.30	15.00
214 LYS CA	-28.14	-34.63	74.23	15.00
214 LYS CB	-27.49	-36.02	74.28	15.00
214 LYS CG	-28.32	-37.14	73.61	15.00
214 LYS CD	-27.43	-38.10	72.81	15.00
214 LYS CE	-26.30	-38.66	73.65	15.00
214 LYS NZ	-25.35	-39.45	72.81	15.00
214 LYS C	-28.02	-33.93	75.57	15.00
214 LYS O	-26.95	-33.45	75.91	15.00
215 MET N	-29.11	-33.79	76.30	15.00
215 MET CA	-29.01	-33.15	77.60	15.00
215 MET CB	-29.60	-31.73	77.56	15.00
215 MET CG	-28.77	-30.73	78.36	15.00
215 MET SD	-29.41	-29.06	78.37	15.00
215 MET CE	-30.41	-29.07	79.82	15.00
215 MET C	-29.66	-33.98	78.71	15.00
215 MET OT1	-30.59	-34.77	78.41	15.00
215 MET OT2	-29.20	-33.85	79.87	15.00
216 HOH OH2	-28.05	-18.06	84.86	15.00
217 HOH OH2	-23.19	-33.36	81.36	15.00
218 HOH OH2	-31.64	-15.80	65.41	15.00
219 HOH OH2	-30.17	-19.91	64.18	15.00
220 HOH OH2	-13.36	-11.60	62.86	15.00
221 HOH OH2	-9.95	-9.46	71.42	15.00
222 HOH OH2	-34.59	-22.68	70.30	15.00
223 HOH OH2	-17.52	-33.99	64.33	15.00
224 HOH OH2	-15.72	-11.02	61.35	15.00
225 HOH OH2	-24.41	-30.51	62.51	15.00
226 HOH OH2	-10.27	-5.38	68.19	15.00
227 HOH OH2	-11.06	-16.84	67.70	15.00
228 HOH OH2	-44.88	-30.73	49.92	15.00
229 HOH OH2	-44.59	-36.65	56.24	15.00
230 HOH OH2	-37.78	-15.40	68.33	15.00
231 HOH OH2	-38.40	-35.66	51.51	15.00
232 HOH OH2	-18.90	-36.86	61.93	15.00
233 HOH OH2	-41.75	-34.32	46.57	15.00
234 HOH OH2	-28.01	-19.38	62.11	15.00

TABLE III

235	HOH	OH2	-21.94	-29.60	62.55	15.00
236	HOH	OH2	-26.15	-8.89	74.53	15.00
237	HOH	OH2	-29.39	-20.71	79.14	15.00
238	HOH	OH2	-30.20	-22.42	84.30	15.00
239	HOH	OH2	-40.59	-13.37	49.72	15.00
240	HOH	OH2	-36.04	-24.57	49.50	15.00
241	HOH	OH2	-46.35	-34.82	56.72	15.00
242	HOH	OH2	-24.71	-3.06	61.99	15.00
243	HOH	OH2	-44.08	-16.56	65.62	15.00
244	HOH	OH2	-25.57	-5.90	65.10	15.00
245	HOH	OH2	-33.44	-27.60	71.31	15.00
246	HOH	OH2	-47.48	-27.33	77.05	15.00
247	HOH	OH2	-14.60	-14.01	81.32	15.00
248	HOH	OH2	-7.93	-18.05	73.48	15.00
249	HOH	OH2	-7.49	-16.70	75.98	15.00
250	HOH	OH2	-26.27	-35.42	59.26	15.00
251	HOH	OH2	-35.15	-10.72	53.73	15.00
252	HOH	OH2	-33.62	-27.20	46.10	15.00
253	HOH	OH2	-40.60	-16.73	45.07	15.00
254	HOH	OH2	-41.25	-34.55	55.94	15.00
255	HOH	OH2	-40.71	-18.20	72.64	15.00
256	HOH	OH2	-32.67	-13.41	60.76	15.00
257	HOH	OH2	-39.61	-9.04	58.76	15.00
258	HOH	OH2	-31.33	-8.54	65.90	15.00
259	HOH	OH2	-31.41	-5.90	63.60	15.00
260	HOH	OH2	-19.54	-8.02	63.36	15.00
261	HOH	OH2	-33.59	-19.88	70.38	15.00
262	HOH	OH2	-32.78	-42.12	66.81	15.00
263	HOH	OH2	-13.22	-22.75	77.99	15.00
264	HOH	OH2	-8.15	-22.46	73.27	15.00
265	HOH	OH2	-9.06	-29.93	75.92	15.00
266	HOH	OH2	-20.77	-33.56	62.36	15.00
267	HOH	OH2	-24.27	-45.12	64.98	15.00
268	HOH	OH2	-11.63	-32.82	70.13	15.00
269	HOH	OH2	-11.87	-26.78	72.10	15.00
270	HOH	OH2	-19.16	-34.47	79.41	15.00
271	HOH	OH2	-22.14	-37.69	70.75	15.00
272	HOH	OH2	-34.50	-24.81	88.02	15.00
273	HOH	OH2	-6.96	-12.16	66.61	15.00
274	HOH	OH2	-7.05	-22.45	69.94	15.00
275	HOH	OH2	-16.95	-20.23	55.91	15.00
276	HOH	OH2	-29.20	-20.58	48.90	15.00
277	HOH	OH2	-25.90	-22.48	45.16	15.00

TABLE III

278	HOH	OH2	-35.36	-37.73	52.91	15.00
279	HOH	OH2	-20.12	-27.71	43.74	15.00
280	HOH	OH2	-38.87	-31.38	41.99	15.00
281	HOH	OH2	-38.13	-30.43	51.07	15.00

TABLE VI

6 ASP CA	-43.81	-24.70	66.29	15.00
6 ASP CB	-44.76	-23.60	65.80	15.00
6 ASP CG	-44.06	-22.25	65.59	15.00
6 ASP OD1	-42.88	-22.10	65.94	15.00
6 ASP OD2	-44.73	-21.33	65.08	15.00
6 ASP C	-43.41	-24.48	67.75	15.00
6 ASP O	-44.26	-24.33	68.63	15.00
7 TYR N	-42.12	-24.54	68.00	15.00
7 TYR CA	-41.60	-24.37	69.34	15.00
7 TYR CB	-40.20	-24.96	69.42	15.00
7 TYR CG	-40.23	-26.49	69.41	15.00
7 TYR CD1	-40.62	-27.20	70.55	15.00
7 TYR CE1	-40.66	-28.57	70.55	15.00
7 TYR CD2	-39.89	-27.21	68.27	15.00
7 TYR CE2	-39.94	-28.60	68.26	15.00
7 TYR CZ	-40.32	-29.27	69.41	15.00
7 TYR OH	-40.40	-30.63	69.42	15.00
7 TYR C	-41.64	-22.94	69.83	15.00
7 TYR O	-41.52	-22.68	71.03	15.00
8 ARG N	-41.85	-22.01	68.90	15.00
8 ARG CA	-41.91	-20.58	69.22	15.00
8 ARG CB	-42.07	-19.74	67.95	15.00
8 ARG CG	-40.84	-19.78	67.04	15.00
8 ARG CD	-41.01	-18.96	65.78	15.00
8 ARG NE	-41.97	-19.57	64.86	15.00
8 ARG CZ	-42.43	-18.97	63.77	15.00
8 ARG NH1	-42.03	-17.75	63.46	15.00
8 ARG NH2	-43.30	-19.60	62.98	15.00
8 ARG C	-43.09	-20.36	70.15	15.00
8 ARG O	-42.95	-19.71	71.18	15.00
9 LYS N	-44.23	-20.95	69.82	15.00
9 LYS CA	-45.41	-20.80	70.64	15.00
9 LYS CB	-46.59	-21.48	69.96	15.00
9 LYS CG	-46.93	-20.90	68.60	15.00
9 LYS CD	-47.74	-21.89	67.79	15.00
9 LYS CE	-48.07	-21.38	66.41	15.00
9 LYS NZ	-48.46	-22.50	65.49	15.00
9 LYS C	-45.16	-21.46	71.99	15.00
9 LYS O	-45.70	-21.01	73.01	15.00
10 LYS N	-44.29	-22.46	71.99	15.00
10 LYS CA	-43.94	-23.25	73.18	15.00
10 LYS CB	-43.34	-24.60	72.77	15.00
10 LYS CG	-44.19	-25.43	71.81	15.00

TABLE VI

10	LYS	CD	-45.03	-26.48	72.52	15.00
10	LYS	CE	-46.23	-25.86	73.25	15.00
10	LYS	NZ	-47.28	-25.31	72.33	15.00
10	LYS	C	-42.97	-22.59	74.15	15.00
10	LYS	O	-42.91	-22.97	75.32	15.00
11	GLY	N	-42.15	-21.66	73.67	15.00
11	GLY	CA	-41.20	-21.02	74.57	15.00
11	GLY	C	-39.83	-21.68	74.55	15.00
11	GLY	O	-39.00	-21.42	75.42	15.00
12	TYR	N	-39.57	-22.49	73.53	15.00
12	TYR	CA	-38.29	-23.18	73.39	15.00
12	TYR	CB	-38.48	-24.53	72.68	15.00
12	TYR	CG	-39.09	-25.67	73.49	15.00
12	TYR	CD1	-40.24	-25.49	74.27	15.00
12	TYR	CE1	-40.82	-26.55	74.95	15.00
12	TYR	CD2	-38.55	-26.95	73.42	15.00
12	TYR	CE2	-39.13	-28.01	74.09	15.00
12	TYR	CZ	-40.26	-27.81	74.85	15.00
12	TYR	OH	-40.86	-28.88	75.47	15.00
12	TYR	C	-37.31	-22.37	72.55	15.00
12	TYR	O	-36.15	-22.73	72.44	15.00
13	VAL	N	-37.78	-21.29	71.94	15.00
13	VAL	CA	-36.94	-20.46	71.07	15.00
13	VAL	CB	-37.56	-20.37	69.65	15.00
13	VAL	CG1	-36.60	-19.70	68.68	15.00
13	VAL	CG2	-37.91	-21.76	69.16	15.00
13	VAL	C	-36.75	-19.06	71.62	15.00
13	VAL	O	-37.70	-18.41	72.02	15.00
14	THR	N	-35.51	-18.61	71.66	15.00
14	THR	CA	-35.21	-17.27	72.15	15.00
14	THR	CB	-33.80	-17.21	72.74	15.00
14	THR	OG1	-32.85	-17.58	71.74	15.00
14	THR	CG2	-33.69	-18.13	73.92	15.00
14	THR	C	-35.31	-16.23	71.02	15.00
14	THR	O	-35.46	-16.59	69.85	15.00
15	PRO	N	-35.25	-14.94	71.35	15.00
15	PRO	CD	-35.15	-14.35	72.71	15.00
15	PRO	CA	-35.34	-13.89	70.34	15.00
15	PRO	CB	-35.15	-12.62	71.16	15.00
15	PRO	CG	-35.72	-12.99	72.50	15.00
15	PRO	C	-34.26	-14.00	69.25	15.00
15	PRO	O	-33.13	-14.41	69.53	15.00
16	VAL	N	-34.61	-13.62	68.02	15.00

TABLE VI

16 VAL CA	-33.69	-13.67	66.89	15.00
16 VAL CB	-34.39	-13.43	65.54	15.00
16 VAL CG1	-33.36	-13.27	64.43	15.00
16 VAL CG2	-35.29	-14.58	65.20	15.00
16 VAL C	-32.56	-12.66	67.05	15.00
16 VAL O	-32.79	-11.47	67.28	15.00
17 LYS N	-31.34	-13.17	66.92	15.00
17 LYS CA	-30.15	-12.36	67.04	15.00
17 LYS CB	-29.13	-13.09	67.91	15.00
17 LYS CG	-29.67	-13.49	69.27	15.00
17 LYS CD	-30.28	-12.30	69.96	15.00
17 LYS CE	-30.93	-12.65	71.28	15.00
17 LYS NZ	-31.68	-11.47	71.83	15.00
17 LYS C	-29.58	-12.08	65.65	15.00
17 LYS O	-30.13	-12.52	64.64	15.00
18 ASN N	-28.48	-11.33	65.60	15.00
18 ASN CA	-27.82	-10.98	64.34	15.00
18 ASN CB	-28.02	-9.49	64.05	15.00
18 ASN CG	-27.42	-9.05	62.72	15.00
18 ASN OD1	-26.35	-9.49	62.32	15.00
18 ASN ND2	-28.11	-8.15	62.03	15.00
18 ASN C	-26.32	-11.27	64.49	15.00
18 ASN O	-25.67	-10.71	65.37	15.00
19 GLN N	-25.79	-12.14	63.63	15.00
19 GLN CA	-24.38	-12.49	63.68	15.00
19 GLN CB	-24.08	-13.76	62.87	15.00
19 GLN CG	-24.55	-13.74	61.41	15.00
19 GLN CD	-24.19	-15.02	60.65	15.00
19 GLN OE1	-25.06	-15.85	60.37	15.00
19 GLN NE2	-22.92	-15.16	60.28	15.00
19 GLN C	-23.43	-11.34	63.29	15.00
19 GLN O	-22.26	-11.34	63.67	15.00
20 GLY N	-23.92	-10.39	62.50	15.00
20 GLY CA	-23.11	-9.25	62.11	15.00
20 GLY C	-22.23	-9.49	60.91	15.00
20 GLY O	-22.71	-9.92	59.87	15.00
21 GLN N	-20.96	-9.14	61.02	15.00
21 GLN CA	-20.02	-9.34	59.92	15.00
21 GLN CB	-19.11	-8.11	59.75	15.00
21 GLN CG	-19.78	-6.87	59.13	15.00
21 GLN CD	-20.32	-7.11	57.72	15.00
21 GLN OE1	-19.57	-7.44	56.79	15.00
21 GLN NE2	-21.62	-6.95	57.55	15.00

TABLE VI

21 GLN C	-19.18	-10.59	60.17	15.00
21 GLN O	-18.39	-11.01	59.33	15.00
22 CYS N	-19.34	-11.17	61.36	15.00
22 CYS CA	-18.63	-12.38	61.75	15.00
22 CYS C	-19.40	-13.60	61.22	15.00
22 CYS O	-20.64	-13.58	61.15	15.00
22 CYS CB	-18.52	-12.41	63.27	15.00
22 CYS SG	-17.94	-13.95	64.05	15.00
23 GLY N	-18.68	-14.63	60.78	15.00
23 GLY CA	-19.32	-15.82	60.25	15.00
23 GLY C	-19.52	-16.87	61.32	15.00
23 GLY O	-19.06	-18.00	61.18	15.00
24 SER N	-20.24	-16.49	62.37	15.00
24 SER CA	-20.52	-17.34	63.52	15.00
24 SER CB	-20.42	-16.49	64.77	15.00
24 SER OG	-21.27	-15.36	64.65	15.00
24 SER C	-21.92	-17.95	63.44	15.00
24 SER O	-22.54	-18.24	64.47	15.00
25 CYS N	-22.40	-18.17	62.23	15.00
25 CYS CA	-23.72	-18.75	62.04	15.00
25 CYS CB	-24.08	-18.74	60.55	15.00
25 CYS SG	-23.06	-19.79	59.52	15.00
25 CYS C	-23.81	-20.15	62.66	15.00
25 CYS O	-24.90	-20.59	63.05	15.00
25 INH C1	-27.01	-9.79	58.47	15.00
25 INH C2	-26.33	-10.46	59.49	15.00
25 INH C3	-25.12	-11.10	59.22	15.00
25 INH C4	-24.57	-11.08	57.94	15.00
25 INH C5	-25.26	-10.40	56.92	15.00
25 INH C6	-26.47	-9.76	57.18	15.00
25 INH C7	-23.25	-11.75	57.65	15.00
25 INH O8	-23.16	-13.18	57.51	15.00
25 INH C9	-22.82	-13.83	56.29	15.00
25 INH C10	-22.10	-13.30	55.22	15.00
25 INH C11	-23.03	-15.93	55.08	15.00
25 INH C12	-22.32	-15.39	54.01	15.00
25 INH C13	-21.85	-14.07	54.07	15.00
25 INH C14	-23.54	-17.29	55.29	15.00
25 INH O15	-24.49	-17.82	54.70	15.00
25 INH N16	-22.71	-17.77	56.29	15.00
25 INH N17	-22.76	-19.07	56.92	15.00
25 INH C18	-23.27	-15.13	56.20	15.00
25 INH C19	-22.05	-19.01	58.26	15.00

TABLE VI

25 INH O20	-21.78	-17.83	58.57	15.00
25 INH C21	-21.27	-30.33	52.84	15.00
25 INH C22	-20.95	-30.49	54.19	15.00
25 INH C23	-20.34	-29.44	54.89	15.00
25 INH C24	-20.03	-28.23	54.25	15.00
25 INH C25	-20.35	-28.09	52.90	15.00
25 INH C26	-20.96	-29.12	52.19	15.00
25 INH C27	-19.35	-27.11	55.01	15.00
25 INH O28	-20.01	-25.85	55.20	15.00
25 INH C29	-20.09	-25.30	56.50	15.00
25 INH O30	-19.34	-25.70	57.40	15.00
25 INH C31	-21.28	-23.64	57.93	15.00
25 INH C32	-21.14	-24.56	59.14	15.00
25 INH C33	-22.16	-25.68	59.35	15.00
25 INH C34	-23.25	-25.62	58.28	15.00
25 INH C35	-21.45	-27.01	59.33	15.00
25 INH C36	-20.52	-22.34	58.22	15.00
25 INH O37	-19.37	-22.35	58.66	15.00
25 INH N38	-21.23	-21.24	57.98	15.00
25 INH N39	-20.81	-19.86	58.17	15.00
25 INH N40	-21.01	-24.34	56.66	15.00
26 TRP N	-22.67	-20.83	62.82	15.00
26 TRP CA	-22.65	-22.16	63.44	15.00
26 TRP CB	-21.35	-22.91	63.12	15.00
26 TRP CG	-20.11	-22.22	63.59	15.00
26 TRP CD2	-19.48	-22.37	64.87	15.00
26 TRP CE2	-18.42	-21.44	64.92	15.00
26 TRP CE3	-19.71	-23.18	65.98	15.00
26 TRP CD1	-19.41	-21.27	62.93	15.00
26 TRP NE1	-18.40	-20.78	63.72	15.00
26 TRP CZ2	-17.59	-21.30	66.03	15.00
26 TRP CZ3	-18.88	-23.05	67.10	15.00
26 TRP CH2	-17.84	-22.11	67.11	15.00
26 TRP C	-22.85	-22.06	64.96	15.00
26 TRP O	-23.57	-22.86	65.55	15.00
27 ALA N	-22.24	-21.04	65.57	15.00
27 ALA CA	-22.33	-20.83	67.01	15.00
27 ALA CB	-21.35	-19.78	67.46	15.00
27 ALA C	-23.74	-20.47	67.45	15.00
27 ALA O	-24.21	-20.91	68.50	15.00
28 PHE N	-24.42	-19.66	66.66	15.00
28 PHE CA	-25.79	-19.27	66.96	15.00
28 PHE CB	-26.23	-18.10	66.07	15.00

TABLE VI

28 PHE CG	-25.67	-16.77	66.49	15.00
28 PHE CD1	-24.46	-16.32	65.99	15.00
28 PHE CD2	-26.35	-15.98	67.42	15.00
28 PHE CE1	-23.92	-15.11	66.41	15.00
28 PHE CE2	-25.81	-14.78	67.84	15.00
28 PHE CZ	-24.60	-14.35	67.34	15.00
28 PHE C	-26.74	-20.47	66.82	15.00
28 PHE O	-27.62	-20.68	67.66	15.00
29 SER N	-26.56	-21.25	65.78	15.00
29 SER CA	-27.40	-22.41	65.55	15.00
29 SER CB	-27.05	-23.08	64.23	15.00
29 SER OG	-27.68	-24.35	64.15	15.00
29 SER C	-27.28	-23.44	66.66	15.00
29 SER O	-28.27	-24.06	67.03	15.00
30 SER N	-26.06	-23.65	67.16	15.00
30 SER CA	-25.79	-24.61	68.22	15.00
30 SER CB	-24.29	-24.72	68.44	15.00
30 SER OG	-23.64	-25.04	67.22	15.00
30 SER C	-26.44	-24.15	69.51	15.00
30 SER O	-27.07	-24.93	70.25	15.00
31 VAL N	-26.25	-22.87	69.80	15.00
31 VAL CA	-26.81	-22.23	70.98	15.00
31 VAL CB	-26.39	-20.75	71.00	15.00
31 VAL CG1	-27.52	-19.85	71.44	15.00
31 VAL CG2	-25.18	-20.58	71.92	15.00
31 VAL C	-28.32	-22.41	70.92	15.00
31 VAL O	-28.95	-22.72	71.94	15.00
32 GLY N	-28.89	-22.27	69.73	15.00
32 GLY CA	-30.32	-22.44	69.56	15.00
32 GLY C	-30.76	-23.83	69.97	15.00
32 GLY O	-31.77	-24.00	70.65	15.00
33 ALA N	-30.00	-24.83	69.55	15.00
33 ALA CA	-30.28	-26.21	69.89	15.00
33 ALA CB	-29.29	-27.14	69.22	15.00
33 ALA C	-30.20	-26.34	71.42	15.00
33 ALA O	-31.19	-26.70	72.06	15.00
34 LEU N	-29.06	-25.98	71.99	15.00
34 LEU CA	-28.87	-26.06	73.44	15.00
34 LEU CB	-27.55	-25.42	73.85	15.00
34 LEU CG	-26.25	-26.10	73.41	15.00
34 LEU CD1	-25.07	-25.21	73.74	15.00
34 LEU CD2	-26.11	-27.45	74.08	15.00
34 LEU C	-30.02	-25.41	74.21	15.00

TABLE VI

34 LEU O	-30.59	-26.01	75.13	15.00
35 GLU N	-30.39	-24.20	73.80	15.00
35 GLU CA	-31.46	-23.44	74.44	15.00
35 GLU CB	-31.63	-22.08	73.77	15.00
35 GLU CG	-30.41	-21.18	73.87	15.00
35 GLU CD	-30.58	-19.86	73.15	15.00
35 GLU OE1	-31.46	-19.76	72.27	15.00
35 GLU OE2	-29.83	-18.92	73.46	15.00
35 GLU C	-32.79	-24.17	74.42	15.00
35 GLU O	-33.51	-24.18	75.42	15.00
36 GLY N	-33.11	-24.77	73.27	15.00
36 GLY CA	-34.35	-25.52	73.13	15.00
36 GLY C	-34.42	-26.67	74.11	15.00
36 GLY O	-35.48	-26.98	74.65	15.00
37 GLN N	-33.28	-27.30	74.37	15.00
37 GLN CA	-33.21	-28.42	75.29	15.00
37 GLN CB	-31.94	-29.22	75.05	15.00
37 GLN CG	-32.00	-30.06	73.80	15.00
37 GLN CD	-33.19	-31.00	73.80	15.00
37 GLN OE1	-33.32	-31.84	74.69	15.00
37 GLN NE2	-34.07	-30.83	72.84	15.00
37 GLN C	-33.28	-27.96	76.74	15.00
37 GLN O	-33.94	-28.58	77.58	15.00
38 LEU N	-32.64	-26.83	77.01	15.00
38 LEU CA	-32.62	-26.25	78.35	15.00
38 LEU CB	-31.77	-24.98	78.37	15.00
38 LEU CG	-31.54	-24.37	79.75	15.00
38 LEU CD1	-30.73	-25.34	80.61	15.00
38 LEU CD2	-30.82	-23.05	79.63	15.00
38 LEU C	-34.04	-25.95	78.83	15.00
38 LEU O	-34.31	-25.95	80.02	15.00
39 LYS N	-34.94	-25.65	77.90	15.00
39 LYS CA	-36.32	-25.38	78.26	15.00
39 LYS CB	-37.04	-24.66	77.12	15.00
39 LYS CG	-38.53	-24.45	77.32	15.00
39 LYS CD	-38.85	-23.47	78.43	15.00
39 LYS CE	-40.35	-23.46	78.70	15.00
39 LYS NZ	-40.71	-22.74	79.94	15.00
39 LYS C	-36.98	-26.72	78.54	15.00
39 LYS O	-37.63	-26.90	79.57	15.00
40 LYS N	-36.73	-27.68	77.65	15.00
40 LYS CA	-37.28	-29.03	77.72	15.00
40 LYS CB	-36.61	-29.90	76.66	15.00

TABLE VI

40 LYS CG	-37.25	-31.25	76.41	15.00
40 LYS CD	-38.51	-31.10	75.61	15.00
40 LYS CE	-39.15	-32.44	75.34	15.00
40 LYS NZ	-38.32	-33.29	74.44	15.00
40 LYS C	-37.07	-29.66	79.08	15.00
40 LYS O	-37.99	-30.28	79.63	15.00
41 LYS N	-35.87	-29.50	79.64	15.00
41 LYS CA	-35.54	-30.10	80.93	15.00
41 LYS CB	-34.07	-30.55	80.94	15.00
41 LYS CG	-33.59	-31.28	79.68	15.00
41 LYS CD	-34.50	-32.44	79.28	15.00
41 LYS CE	-34.05	-33.08	77.96	15.00
41 LYS NZ	-35.06	-34.05	77.42	15.00
41 LYS C	-35.79	-29.20	82.14	15.00
41 LYS O	-36.48	-29.59	83.09	15.00
42 THR N	-35.20	-28.01	82.11	15.00
42 THR CA	-35.30	-27.03	83.19	15.00
42 THR CB	-34.20	-25.98	82.99	15.00
42 THR OG1	-32.95	-26.64	82.85	15.00
42 THR CG2	-34.13	-25.03	84.17	15.00
42 THR C	-36.64	-26.32	83.38	15.00
42 THR O	-36.96	-25.86	84.48	15.00
43 GLY N	-37.43	-26.23	82.31	15.00
43 GLY CA	-38.70	-25.53	82.38	15.00
43 GLY C	-38.52	-24.01	82.29	15.00
43 GLY O	-39.48	-23.25	82.34	15.00
44 LYS N	-37.27	-23.57	82.16	15.00
44 LYS CA	-36.94	-22.15	82.05	15.00
44 LYS CB	-36.25	-21.65	83.33	15.00
44 LYS CG	-37.19	-21.45	84.50	15.00
44 LYS CD	-36.45	-21.05	85.78	15.00
44 LYS CE	-35.71	-22.21	86.39	15.00
44 LYS NZ	-36.62	-23.38	86.62	15.00
44 LYS C	-35.98	-21.98	80.87	15.00
44 LYS O	-35.10	-22.82	80.66	15.00
45 LEU N	-36.17	-20.92	80.10	15.00
45 LEU CA	-35.33	-20.65	78.93	15.00
45 LEU CB	-36.23	-20.21	77.77	15.00
45 LEU CG	-35.64	-20.07	76.38	15.00
45 LEU CD1	-35.28	-21.42	75.82	15.00
45 LEU CD2	-36.67	-19.42	75.52	15.00
45 LEU C	-34.33	-19.56	79.25	15.00
45 LEU O	-34.59	-18.70	80.09	15.00

TABLE VI

46 LEU N	-33.18	-19.57	78.58	15.00
46 LEU CA	-32.16	-18.56	78.80	15.00
46 LEU CB	-31.30	-18.93	80.01	15.00
46 LEU CG	-30.51	-17.78	80.61	15.00
46 LEU CD1	-31.46	-16.70	81.06	15.00
46 LEU CD2	-29.69	-18.27	81.78	15.00
46 LEU C	-31.27	-18.40	77.56	15.00
46 LEU O	-31.02	-19.36	76.85	15.00
47 ASN N	-30.83	-17.17	77.29	15.00
47 ASN CA	-29.98	-16.89	76.13	15.00
47 ASN CB	-29.92	-15.38	75.84	15.00
47 ASN CG	-31.27	-14.80	75.53	15.00
47 ASN OD1	-31.93	-14.22	76.41	15.00
47 ASN ND2	-31.71	-14.94	74.29	15.00
47 ASN C	-28.57	-17.36	76.39	15.00
47 ASN O	-27.91	-16.86	77.30	15.00
48 LEU N	-28.10	-18.32	75.61	15.00
48 LEU CA	-26.75	-18.84	75.78	15.00
48 LEU CB	-26.70	-20.31	75.39	15.00
48 LEU CG	-27.60	-21.19	76.26	15.00
48 LEU CD1	-27.18	-22.64	76.10	15.00
48 LEU CD2	-27.50	-20.77	77.73	15.00
48 LEU C	-25.77	-18.04	74.98	15.00
48 LEU O	-26.14	-17.34	74.04	15.00
49 SER N	-24.50	-18.13	75.34	15.00
49 SER CA	-23.47	-17.36	74.67	15.00
49 SER CB	-22.34	-17.06	75.64	15.00
49 SER OG	-21.34	-16.25	75.03	15.00
49 SER C	-22.89	-17.98	73.40	15.00
49 SER O	-22.29	-19.06	73.45	15.00
50 PRO N	-23.07	-17.31	72.24	15.00
50 PRO CD	-24.05	-16.24	72.05	15.00
50 PRO CA	-22.55	-17.77	70.95	15.00
50 PRO CB	-23.37	-16.96	69.95	15.00
50 PRO CG	-24.61	-16.59	70.71	15.00
50 PRO C	-21.09	-17.37	70.86	15.00
50 PRO O	-20.29	-18.01	70.19	15.00
51 GLN N	-20.74	-16.27	71.52	15.00
51 GLN CA	-19.37	-15.78	71.56	15.00
51 GLN CB	-19.30	-14.45	72.33	15.00
51 GLN CG	-17.93	-13.77	72.34	15.00
51 GLN CD	-17.55	-13.17	71.00	15.00
51 GLN OE1	-18.39	-12.57	70.31	15.00

TABLE VI

51 GLN NE2	-16.29	-13.29	70.64	15.00
51 GLN C	-18.53	-16.82	72.26	15.00
51 GLN O	-17.45	-17.17	71.80	15.00
52 ASN N	-19.03	-17.33	73.38	15.00
52 ASN CA	-18.30	-18.34	74.14	15.00
52 ASN CB	-19.20	-18.91	75.24	15.00
52 ASN CG	-18.51	-19.98	76.10	15.00
52 ASN OD1	-19.13	-20.54	76.99	15.00
52 ASN ND2	-17.23	-20.22	75.86	15.00
52 ASN C	-17.86	-19.45	73.19	15.00
52 ASN O	-16.70	-19.87	73.22	15.00
53 LEU N	-18.76	-19.88	72.32	15.00
53 LEU CA	-18.42	-20.92	71.38	15.00
53 LEU CB	-19.66	-21.39	70.63	15.00
53 LEU CG	-20.68	-22.14	71.49	15.00
53 LEU CD1	-21.63	-22.88	70.59	15.00
53 LEU CD2	-19.98	-23.13	72.38	15.00
53 LEU C	-17.35	-20.41	70.42	15.00
53 LEU O	-16.28	-21.02	70.31	15.00
54 VAL N	-17.61	-19.27	69.79	15.00
54 VAL CA	-16.68	-18.63	68.86	15.00
54 VAL CB	-17.16	-17.18	68.52	15.00
54 VAL CG1	-16.02	-16.35	67.96	15.00
54 VAL CG2	-18.31	-17.21	67.54	15.00
54 VAL C	-15.24	-18.57	69.37	15.00
54 VAL O	-14.31	-18.91	68.66	15.00
55 ASP N	-15.07	-18.14	70.61	15.00
55 ASP CA	-13.75	-18.00	71.21	15.00
55 ASP CB	-13.78	-16.96	72.33	15.00
55 ASP CG	-14.29	-15.61	71.87	15.00
55 ASP OD1	-14.16	-15.30	70.67	15.00
55 ASP OD2	-14.79	-14.85	72.72	15.00
55 ASP C	-13.10	-19.26	71.77	15.00
55 ASP O	-11.88	-19.33	71.86	15.00
56 CYS N	-13.89	-20.25	72.17	15.00
56 CYS CA	-13.31	-21.45	72.77	15.00
56 CYS C	-13.25	-22.75	71.96	15.00
56 CYS O	-12.44	-23.62	72.27	15.00
56 CYS CB	-13.98	-21.73	74.11	15.00
56 CYS SG	-14.30	-20.24	75.11	15.00
57 VAL N	-14.09	-22.89	70.94	15.00
57 VAL CA	-14.08	-24.13	70.16	15.00
57 VAL CB	-15.43	-24.34	69.42	15.00

TABLE VI

57 VAL CG1	-15.47	-25.73	68.80	15.00
57 VAL CG2	-16.59	-24.17	70.38	15.00
57 VAL C	-12.91	-24.19	69.18	15.00
57 VAL O	-13.08	-24.04	67.98	15.00
58 SER N	-11.71	-24.46	69.70	15.00
58 SER CA	-10.50	-24.55	68.89	15.00
58 SER CB	-9.34	-25.09	69.72	15.00
58 SER OG	-9.08	-24.27	70.85	15.00
58 SER C	-10.61	-25.37	67.62	15.00
58 SER O	-9.84	-25.18	66.70	15.00
59 GLU N	-11.57	-26.29	67.56	15.00
59 GLU CA	-11.71	-27.13	66.38	15.00
59 GLU CB	-12.49	-28.41	66.73	15.00
59 GLU CG	-11.81	-29.30	67.75	15.00
59 GLU CD	-11.90	-28.75	69.16	15.00
59 GLU OE1	-12.96	-28.18	69.51	15.00
59 GLU OE2	-10.92	-28.91	69.91	15.00
59 GLU C	-12.39	-26.41	65.23	15.00
59 GLU O	-12.46	-26.91	64.11	15.00
60 ASN N	-12.93	-25.24	65.53	15.00
60 ASN CA	-13.61	-24.41	64.53	15.00
60 ASN CB	-14.99	-24.01	65.03	15.00
60 ASN CG	-15.97	-25.16	65.02	15.00
60 ASN OD1	-17.03	-25.09	65.63	15.00
60 ASN ND2	-15.62	-26.23	64.31	15.00
60 ASN C	-12.75	-23.19	64.27	15.00
60 ASN O	-11.79	-22.94	64.98	15.00
61 ASP N	-13.12	-22.41	63.25	15.00
61 ASP CA	-12.36	-21.23	62.88	15.00
61 ASP CB	-12.21	-21.20	61.35	15.00
61 ASP CG	-10.99	-20.43	60.90	15.00
61 ASP OD1	-10.38	-19.70	61.71	15.00
61 ASP OD2	-10.63	-20.55	59.71	15.00
61 ASP C	-12.92	-19.89	63.39	15.00
61 ASP O	-12.71	-18.86	62.76	15.00
62 GLY N	-13.61	-19.89	64.52	15.00
62 GLY CA	-14.16	-18.66	65.06	15.00
62 GLY C	-15.11	-17.97	64.10	15.00
62 GLY O	-16.17	-18.50	63.79	15.00
63 CYS N	-14.73	-16.79	63.62	15.00
63 CYS CA	-15.56	-16.06	62.67	15.00
63 CYS C	-15.39	-16.55	61.24	15.00
63 CYS O	-16.01	-16.03	60.31	15.00

TABLE VI

63 CYS CB	-15.28	-14.56	62.73	15.00
63 CYS SG	-15.94	-13.72	64.20	15.00
64 GLY N	-14.52	-17.54	61.06	15.00
64 GLY CA	-14.28	-18.09	59.74	15.00
64 GLY C	-15.24	-19.23	59.47	15.00
64 GLY O	-15.42	-19.63	58.32	15.00
65 GLY N	-15.85	-19.77	60.52	15.00
65 GLY CA	-16.79	-20.86	60.33	15.00
65 GLY C	-16.54	-22.03	61.25	15.00
65 GLY O	-15.56	-22.04	62.00	15.00
66 GLY N	-17.42	-23.02	61.19	15.00
66 GLY CA	-17.29	-24.19	62.03	15.00
66 GLY C	-18.50	-25.10	61.96	15.00
66 GLY O	-19.48	-24.76	61.32	15.00
67 TYR N	-18.43	-26.25	62.62	15.00
67 TYR CA	-19.53	-27.20	62.62	15.00
67 TYR CB	-19.02	-28.60	62.32	15.00
67 TYR CG	-18.35	-28.77	60.99	15.00
67 TYR CD1	-19.08	-29.16	59.86	15.00
67 TYR CE1	-18.46	-29.38	58.65	15.00
67 TYR CD2	-16.98	-28.59	60.86	15.00
67 TYR CE2	-16.36	-28.81	59.65	15.00
67 TYR CZ	-17.10	-29.20	58.55	15.00
67 TYR OH	-16.46	-29.41	57.35	15.00
67 TYR C	-20.23	-27.22	63.97	15.00
67 TYR O	-19.59	-27.04	65.00	15.00
68 MET N	-21.52	-27.51	63.96	15.00
68 MET CA	-22.31	-27.57	65.19	15.00
68 MET CB	-23.81	-27.69	64.91	15.00
68 MET CG	-24.46	-26.48	64.23	15.00
68 MET SD	-24.10	-26.27	62.47	15.00
68 MET CE	-25.07	-27.56	61.75	15.00
68 MET C	-21.86	-28.72	66.09	15.00
68 MET O	-21.76	-28.56	67.30	15.00
69 THR N	-21.54	-29.86	65.49	15.00
69 THR CA	-21.10	-31.02	66.26	15.00
69 THR CB	-20.78	-32.22	65.35	15.00
69 THR OG1	-20.01	-31.77	64.24	15.00
69 THR CG2	-22.06	-32.86	64.85	15.00
69 THR C	-19.88	-30.71	67.11	15.00
69 THR O	-19.77	-31.19	68.25	15.00
70 ASN N	-18.97	-29.89	66.59	15.00
70 ASN CA	-17.77	-29.52	67.33	15.00

TABLE VI

70 ASN CB	-16.79	-28.76	66.46	15.00
70 ASN CG	-15.98	-29.65	65.58	15.00
70 ASN OD1	-15.42	-29.19	64.60	15.00
70 ASN ND2	-15.89	-30.93	65.92	15.00
70 ASN C	-18.11	-28.66	68.55	15.00
70 ASN O	-17.46	-28.77	69.59	15.00
71 ALA N	-19.12	-27.80	68.40	15.00
71 ALA CA	-19.57	-26.91	69.47	15.00
71 ALA CB	-20.58	-25.91	68.94	15.00
71 ALA C	-20.15	-27.71	70.63	15.00
71 ALA O	-19.80	-27.50	71.78	15.00
72 PHE N	-21.03	-28.66	70.31	15.00
72 PHE CA	-21.64	-29.51	71.33	15.00
72 PHE CB	-22.57	-30.54	70.69	15.00
72 PHE CG	-23.72	-29.93	69.96	15.00
72 PHE CD1	-24.28	-28.73	70.39	15.00
72 PHE CD2	-24.24	-30.55	68.84	15.00
72 PHE CE1	-25.33	-28.16	69.70	15.00
72 PHE CE2	-25.30	-29.98	68.15	15.00
72 PHE CZ	-25.84	-28.78	68.58	15.00
72 PHE C	-20.53	-30.25	72.07	15.00
72 PHE O	-20.43	-30.18	73.31	15.00
73 GLN N	-19.67	-30.90	71.31	15.00
73 GLN CA	-18.56	-31.66	71.86	15.00
73 GLN CB	-17.68	-32.20	70.72	15.00
73 GLN CG	-16.78	-33.40	71.09	15.00
73 GLN CD	-17.54	-34.73	71.21	15.00
73 GLN OE1	-17.47	-35.58	70.31	15.00
73 GLN NE2	-18.21	-34.94	72.35	15.00
73 GLN C	-17.76	-30.78	72.84	15.00
73 GLN O	-17.33	-31.25	73.89	15.00
74 TYR N	-17.62	-29.50	72.53	15.00
74 TYR CA	-16.89	-28.59	73.40	15.00
74 TYR CB	-16.70	-27.22	72.75	15.00
74 TYR CG	-16.35	-26.13	73.74	15.00
74 TYR CD1	-15.09	-26.05	74.30	15.00
74 TYR CE1	-14.77	-25.07	75.22	15.00
74 TYR CD2	-17.30	-25.18	74.12	15.00
74 TYR CE2	-17.00	-24.19	75.04	15.00
74 TYR CZ	-15.73	-24.14	75.59	15.00
74 TYR OH	-15.42	-23.15	76.51	15.00
74 TYR C	-17.58	-28.38	74.73	15.00
74 TYR O	-16.93	-28.39	75.78	15.00

TABLE VI

75 VAL N	-18.88	-28.12	74.67	15.00
75 VAL CA	-19.68	-27.89	75.88	15.00
75 VAL CB	-21.15	-27.58	75.52	15.00
75 VAL CG1	-21.95	-27.27	76.78	15.00
75 VAL CG2	-21.22	-26.39	74.55	15.00
75 VAL C	-19.62	-29.10	76.80	15.00
75 VAL O	-19.60	-28.96	78.03	15.00
76 GLN N	-19.59	-30.29	76.21	15.00
76 GLN CA	-19.51	-31.51	76.98	15.00
76 GLN CB	-19.75	-32.69	76.05	15.00
76 GLN CG	-19.79	-34.05	76.69	15.00
76 GLN CD	-19.56	-35.13	75.66	15.00
76 GLN OE1	-20.03	-35.04	74.53	15.00
76 GLN NE2	-18.78	-36.13	76.03	15.00
76 GLN C	-18.14	-31.60	77.64	15.00
76 GLN O	-18.03	-31.59	78.86	15.00
77 LYS N	-17.08	-31.61	76.84	15.00
77 LYS CA	-15.72	-31.70	77.36	15.00
77 LYS CB	-14.70	-31.55	76.22	15.00
77 LYS CG	-13.27	-31.34	76.69	15.00
77 LYS CD	-12.32	-31.10	75.51	15.00
77 LYS CE	-10.89	-30.81	75.97	15.00
77 LYS NZ	-10.30	-31.95	76.76	15.00
77 LYS C	-15.45	-30.64	78.42	15.00
77 LYS O	-14.81	-30.91	79.45	15.00
78 ASN N	-15.92	-29.42	78.17	15.00
78 ASN CA	-15.74	-28.29	79.06	15.00
78 ASN CB	-15.98	-27.00	78.28	15.00
78 ASN CG	-15.69	-25.76	79.10	15.00
78 ASN OD1	-14.58	-25.59	79.62	15.00
78 ASN ND2	-16.67	-24.87	79.19	15.00
78 ASN C	-16.68	-28.34	80.25	15.00
78 ASN O	-16.42	-27.72	81.28	15.00
79 ARG N	-17.79	-29.06	80.11	15.00
79 ARG CA	-18.78	-29.18	81.16	15.00
79 ARG CB	-18.14	-29.76	82.43	15.00
79 ARG CG	-17.67	-31.20	82.26	15.00
79 ARG CD	-16.65	-31.59	83.33	15.00
79 ARG NE	-17.15	-31.38	84.68	15.00
79 ARG CZ	-18.16	-32.06	85.22	15.00
79 ARG NH1	-18.78	-33.03	84.55	15.00
79 ARG NH2	-18.62	-31.70	86.43	15.00
79 ARG C	-19.45	-27.84	81.45	15.00

TABLE VI

79 ARG O	-19.31	-27.30	82.55	15.00
80 GLY N	-20.13	-27.28	80.45	15.00
80 GLY CA	-20.82	-26.02	80.66	15.00
80 GLY C	-20.62	-24.91	79.64	15.00
80 GLY O	-19.56	-24.82	79.00	15.00
81 ILE N	-21.64	-24.08	79.48	15.00
81 ILE CA	-21.59	-22.95	78.57	15.00
81 ILE CB	-22.30	-23.23	77.22	15.00
81 ILE CG2	-23.77	-23.52	77.45	15.00
81 ILE CG1	-22.10	-22.05	76.27	15.00
81 ILE CD1	-22.84	-22.16	74.96	15.00
81 ILE C	-22.24	-21.75	79.25	15.00
81 ILE O	-23.28	-21.89	79.90	15.00
82 ASP N	-21.61	-20.59	79.11	15.00
82 ASP CA	-22.11	-19.37	79.71	15.00
82 ASP CB	-21.03	-18.29	79.64	15.00
82 ASP CG	-19.90	-18.53	80.58	15.00
82 ASP OD1	-18.82	-17.98	80.34	15.00
82 ASP OD2	-20.09	-19.26	81.58	15.00
82 ASP C	-23.36	-18.81	79.09	15.00
82 ASP O	-23.69	-19.07	77.93	15.00
83 SER N	-24.07	-18.02	79.89	15.00
83 SER CA	-25.27	-17.36	79.44	15.00
83 SER CB	-26.09	-16.90	80.64	15.00
83 SER OG	-25.27	-16.23	81.59	15.00
83 SER C	-24.75	-16.15	78.66	15.00
83 SER O	-23.57	-15.79	78.79	15.00
84 GLU N	-25.61	-15.54	77.86	15.00
84 GLU CA	-25.25	-14.36	77.07	15.00
84 GLU CB	-26.46	-13.84	76.31	15.00
84 GLU CG	-26.17	-12.64	75.43	15.00
84 GLU CD	-25.31	-12.99	74.24	15.00
84 GLU OE1	-24.08	-12.98	74.38	15.00
84 GLU OE2	-25.87	-13.29	73.17	15.00
84 GLU C	-24.70	-13.27	77.99	15.00
84 GLU O	-23.53	-12.89	77.88	15.00
85 ASP N	-25.51	-12.82	78.94	15.00
85 ASP CA	-25.09	-11.79	79.87	15.00
85 ASP CB	-26.13	-11.60	80.99	15.00
85 ASP CG	-25.66	-10.63	82.08	15.00
85 ASP OD1	-25.92	-10.88	83.29	15.00
85 ASP OD2	-25.03	-9.60	81.73	15.00
85 ASP C	-23.72	-12.09	80.49	15.00

TABLE VI

85 ASP O	-22.91	-11.18	80.65	15.00
86 ALA N	-23.45	-13.34	80.81	15.00
86 ALA CA	-22.18	-13.67	81.44	15.00
86 ALA CB	-22.25	-15.05	82.03	15.00
86 ALA C	-21.01	-13.56	80.47	15.00
86 ALA O	-19.91	-13.17	80.86	15.00
87 TYR N	-21.26	-13.89	79.21	15.00
87 TYR CA	-20.23	-13.85	78.18	15.00
87 TYR CB	-19.77	-15.27	77.87	15.00
87 TYR CG	-18.42	-15.39	77.19	15.00
87 TYR CD1	-17.96	-14.41	76.30	15.00
87 TYR CE1	-16.74	-14.56	75.65	15.00
87 TYR CD2	-17.62	-16.52	77.40	15.00
87 TYR CE2	-16.40	-16.67	76.76	15.00
87 TYR CZ	-15.96	-15.69	75.88	15.00
87 TYR OH	-14.75	-15.83	75.25	15.00
87 TYR C	-20.93	-13.23	76.97	15.00
87 TYR O	-21.57	-13.94	76.19	15.00
88 PRO N	-20.90	-11.90	76.86	15.00
88 PRO CD	-20.42	-10.97	77.90	15.00
88 PRO CA	-21.52	-11.15	75.78	15.00
88 PRO CB	-21.33	-9.70	76.23	15.00
88 PRO CG	-21.34	-9.81	77.71	15.00
88 PRO C	-20.91	-11.38	74.39	15.00
88 PRO O	-19.74	-11.74	74.25	15.00
89 TYR N	-21.73	-11.12	73.38	15.00
89 TYR CA	-21.35	-11.29	71.99	15.00
89 TYR CB	-22.56	-11.78	71.18	15.00
89 TYR CG	-22.24	-12.15	69.76	15.00
89 TYR CD1	-21.38	-13.20	69.47	15.00
89 TYR CE1	-21.06	-13.53	68.17	15.00
89 TYR CD2	-22.78	-11.44	68.70	15.00
89 TYR CE2	-22.47	-11.76	67.39	15.00
89 TYR CZ	-21.61	-12.79	67.13	15.00
89 TYR OH	-21.27	-13.08	65.83	15.00
89 TYR C	-20.85	-9.95	71.48	15.00
89 TYR O	-21.52	-8.92	71.64	15.00
90 VAL N	-19.65	-9.94	70.91	15.00
90 VAL CA	-19.07	-8.71	70.39	15.00
90 VAL CB	-17.75	-8.36	71.12	15.00
90 VAL CG1	-17.97	-8.36	72.62	15.00
90 VAL CG2	-16.65	-9.33	70.74	15.00
90 VAL C	-18.88	-8.78	68.87	15.00

TABLE VI

90 VAL O	-18.54	-7.78	68.23	15.00
91 GLY N	-19.08	-9.96	68.30	15.00
91 GLY CA	-18.95	-10.12	66.86	15.00
91 GLY C	-17.55	-10.23	66.27	15.00
91 GLY O	-17.34	-9.87	65.12	15.00
92 GLN N	-16.61	-10.80	67.01	15.00
92 GLN CA	-15.24	-10.95	66.50	15.00
92 GLN CB	-14.56	-9.58	66.41	15.00
92 GLN CG	-14.68	-8.72	67.67	15.00
92 GLN CD	-13.59	-7.67	67.79	15.00
92 GLN OE1	-12.77	-7.72	68.72	15.00
92 GLN NE2	-13.56	-6.72	66.85	15.00
92 GLN C	-14.45	-11.86	67.43	15.00
92 GLN O	-14.78	-11.97	68.62	15.00
93 GLU N	-13.43	-12.52	66.89	15.00
93 GLU CA	-12.64	-13.42	67.71	15.00
93 GLU CB	-11.68	-14.28	66.89	15.00
93 GLU CG	-12.31	-15.10	65.78	15.00
93 GLU CD	-11.63	-14.87	64.44	15.00
93 GLU OE1	-11.94	-15.61	63.48	15.00
93 GLU OE2	-10.78	-13.94	64.33	15.00
93 GLU C	-11.84	-12.62	68.71	15.00
93 GLU O	-11.41	-11.49	68.44	15.00
94 GLU N	-11.61	-13.26	69.85	15.00
94 GLU CA	-10.88	-12.70	70.98	15.00
94 GLU CB	-11.81	-11.81	71.79	15.00
94 GLU CG	-13.19	-12.42	71.93	15.00
94 GLU CD	-14.06	-11.70	72.92	15.00
94 GLU OE1	-13.99	-10.45	72.96	15.00
94 GLU OE2	-14.83	-12.38	73.64	15.00
94 GLU C	-10.52	-13.92	71.80	15.00
94 GLU O	-10.89	-15.02	71.45	15.00
95 SER N	-9.81	-13.73	72.91	15.00
95 SER CA	-9.43	-14.85	73.75	15.00
95 SER CB	-8.32	-14.42	74.71	15.00
95 SER OG	-7.20	-13.94	73.98	15.00
95 SER C	-10.62	-15.42	74.52	15.00
95 SER O	-11.48	-14.67	75.02	15.00
96 CYS N	-10.69	-16.75	74.57	15.00
96 CYS CA	-11.76	-17.45	75.28	15.00
96 CYS C	-11.74	-16.96	76.71	15.00
96 CYS O	-10.73	-17.09	77.42	15.00
96 CYS CB	-11.53	-18.97	75.20	15.00

TABLE VI

96 CYS SG	-12.62	-20.03	76.22	15.00
97 MET N	-12.85	-16.38	77.14	15.00
97 MET CA	-12.96	-15.85	78.49	15.00
97 MET CB	-13.32	-14.36	78.39	15.00
97 MET CG	-12.29	-13.51	77.69	15.00
97 MET SD	-13.01	-11.98	77.03	15.00
97 MET CE	-14.07	-11.44	78.40	15.00
97 MET C	-14.03	-16.60	79.28	15.00
97 MET O	-14.87	-15.99	79.96	15.00
98 TYR N	-13.98	-17.93	79.21	15.00
98 TYR CA	-14.96	-18.74	79.91	15.00
98 TYR CB	-14.69	-20.23	79.71	15.00
98 TYR CG	-15.74	-21.10	80.34	15.00
98 TYR CD1	-17.08	-20.99	79.97	15.00
98 TYR CE1	-18.07	-21.74	80.59	15.00
98 TYR CD2	-15.41	-22.00	81.36	15.00
98 TYR CE2	-16.40	-22.76	81.98	15.00
98 TYR CZ	-17.72	-22.62	81.60	15.00
98 TYR OH	-18.70	-23.34	82.23	15.00
98 TYR C	-15.03	-18.43	81.39	15.00
98 TYR O	-14.01	-18.38	82.08	15.00
99 ASN N	-16.25	-18.27	81.88	15.00
99 ASN CA	-16.49	-17.97	83.28	15.00
99 ASN CB	-17.29	-16.66	83.38	15.00
99 ASN CG	-17.66	-16.33	84.80	15.00
99 ASN OD1	-16.88	-16.57	85.74	15.00
99 ASN ND2	-18.85	-15.79	84.99	15.00
99 ASN C	-17.28	-19.10	83.92	15.00
99 ASN O	-18.51	-19.16	83.78	15.00
100 PRO N	-16.60	-19.99	84.67	15.00
100 PRO CD	-15.22	-19.88	85.16	15.00
100 PRO CA	-17.29	-21.11	85.32	15.00
100 PRO CB	-16.20	-21.72	86.20	15.00
100 PRO CG	-15.31	-20.55	86.51	15.00
100 PRO C	-18.45	-20.63	86.16	15.00
100 PRO O	-19.51	-21.24	86.15	15.00
101 THR N	-18.28	-19.50	86.84	15.00
101 THR CA	-19.33	-18.95	87.68	15.00
101 THR CB	-18.86	-17.68	88.45	15.00
101 THR OG1	-18.71	-16.57	87.55	15.00
101 THR CG2	-17.51	-17.93	89.13	15.00
101 THR C	-20.55	-18.59	86.82	15.00
101 THR O	-21.68	-18.56	87.32	15.00

TABLE VI

102 GLY N	-20.32	-18.34	85.54	15.00
102 GLY CA	-21.40	-17.98	84.64	15.00
102 GLY C	-22.06	-19.12	83.88	15.00
102 GLY O	-22.92	-18.86	83.03	15.00
103 LYS N	-21.65	-20.36	84.12	15.00
103 LYS CA	-22.24	-21.50	83.42	15.00
103 LYS CB	-21.72	-22.83	83.98	15.00
103 LYS CG	-22.32	-24.05	83.29	15.00
103 LYS CD	-22.10	-25.33	84.06	15.00
103 LYS CE	-22.96	-25.41	85.35	15.00
103 LYS NZ	-24.41	-25.79	85.14	15.00
103 LYS C	-23.75	-21.49	83.57	15.00
103 LYS O	-24.26	-21.26	84.67	15.00
104 ALA N	-24.47	-21.73	82.48	15.00
104 ALA CA	-25.93	-21.75	82.53	15.00
104 ALA CB	-26.51	-20.51	81.87	15.00
104 ALA C	-26.52	-22.99	81.89	15.00
104 ALA O	-27.73	-23.15	81.87	15.00
105 ALA N	-25.66	-23.87	81.38	15.00
105 ALA CA	-26.11	-25.10	80.75	15.00
105 ALA CB	-26.84	-24.78	79.44	15.00
105 ALA C	-24.95	-26.03	80.46	15.00
105 ALA O	-23.79	-25.67	80.62	15.00
106 LYS N	-25.28	-27.26	80.07	15.00
106 LYS CA	-24.29	-28.25	79.70	15.00
106 LYS CB	-23.55	-28.80	80.92	15.00
106 LYS CG	-24.41	-29.35	82.04	15.00
106 LYS CD	-23.54	-29.64	83.27	15.00
106 LYS CE	-22.40	-30.62	82.95	15.00
106 LYS NZ	-21.34	-30.67	84.03	15.00
106 LYS C	-24.99	-29.36	78.93	15.00
106 LYS O	-26.21	-29.30	78.75	15.00
107 CYS N	-24.23	-30.30	78.39	15.00
107 CYS CA	-24.82	-31.40	77.64	15.00
107 CYS CB	-25.06	-30.99	76.19	15.00
107 CYS SG	-23.58	-30.95	75.18	15.00
107 CYS C	-23.91	-32.61	77.68	15.00
107 CYS O	-22.75	-32.49	78.06	15.00
108 ARG N	-24.43	-33.77	77.32	15.00
108 ARG CA	-23.64	-35.00	77.33	15.00
108 ARG CB	-24.12	-35.97	78.42	15.00
108 ARG CG	-25.63	-36.03	78.64	15.00
108 ARG CD	-26.27	-37.28	78.04	15.00

TABLE VI

108 ARG NE	-27.73	-37.21	78.14	15.00
108 ARG CZ	-28.57	-38.06	77.54	15.00
108 ARG NH1	-28.09	-39.05	76.80	15.00
108 ARG NH2	-29.88	-37.94	77.72	15.00
108 ARG C	-23.55	-35.70	75.97	15.00
108 ARG O	-23.77	-36.91	75.85	15.00
109 GLY N	-23.19	-34.93	74.94	15.00
109 GLY CA	-23.06	-35.50	73.61	15.00
109 GLY C	-24.08	-34.95	72.65	15.00
109 GLY O	-24.81	-34.01	72.97	15.00
110 TYR N	-24.16	-35.57	71.48	15.00
110 TYR CA	-25.07	-35.16	70.42	15.00
110 TYR CB	-24.41	-34.09	69.55	15.00
110 TYR CG	-23.10	-34.53	68.92	15.00
110 TYR CD1	-21.91	-34.49	69.64	15.00
110 TYR CE1	-20.71	-34.90	69.08	15.00
110 TYR CD2	-23.06	-34.99	67.62	15.00
110 TYR CE2	-21.87	-35.41	67.04	15.00
110 TYR CZ	-20.70	-35.35	67.77	15.00
110 TYR OH	-19.52	-35.75	67.18	15.00
110 TYR C	-25.39	-36.37	69.57	15.00
110 TYR O	-24.80	-37.44	69.77	15.00
111 ARG N	-26.29	-36.20	68.61	15.00
111 ARG CA	-26.69	-37.28	67.73	15.00
111 ARG CB	-27.96	-37.95	68.26	15.00
111 ARG CG	-27.84	-38.48	69.67	15.00
111 ARG CD	-29.18	-39.01	70.20	15.00
111 ARG NE	-29.77	-40.08	69.39	15.00
111 ARG CZ	-29.16	-41.20	69.02	15.00
111 ARG NH1	-29.81	-42.09	68.27	15.00
111 ARG NH2	-27.91	-41.45	69.40	15.00
111 ARG C	-26.98	-36.73	66.35	15.00
111 ARG O	-27.99	-36.05	66.17	15.00
112 GLU N	-26.10	-36.96	65.39	15.00
112 GLU CA	-26.32	-36.48	64.03	15.00
112 GLU CB	-25.09	-36.71	63.15	15.00
112 GLU CG	-23.91	-35.81	63.46	15.00
112 GLU CD	-23.40	-35.09	62.22	15.00
112 GLU OE1	-24.13	-34.21	61.69	15.00
112 GLU OE2	-22.27	-35.41	61.77	15.00
112 GLU C	-27.50	-37.23	63.45	15.00
112 GLU O	-27.70	-38.41	63.76	15.00
113 ILE N	-28.29	-36.55	62.64	15.00

TABLE VI

113	ILE	CA	-29.46	-37.15	62.02	15.00
113	ILE	CB	-30.51	-36.04	61.71	15.00
113	ILE	CG2	-31.75	-36.60	61.05	15.00
113	ILE	CG1	-30.92	-35.38	63.02	15.00
113	ILE	CD1	-31.95	-34.32	62.87	15.00
113	ILE	C	-28.95	-37.84	60.75	15.00
113	ILE	O	-27.93	-37.44	60.20	15.00
114	PRO	N	-29.60	-38.95	60.34	15.00
114	PRO	CD	-30.69	-39.67	61.02	15.00
114	PRO	CA	-29.17	-39.68	59.14	15.00
114	PRO	CB	-30.28	-40.72	58.97	15.00
114	PRO	CG	-30.62	-41.05	60.38	15.00
114	PRO	C	-29.04	-38.79	57.93	15.00
114	PRO	O	-30.00	-38.17	57.47	15.00
115	GLU	N	-27.82	-38.75	57.41	15.00
115	GLU	CA	-27.50	-37.92	56.26	15.00
115	GLU	CB	-26.12	-38.30	55.74	15.00
115	GLU	CG	-25.58	-37.36	54.68	15.00
115	GLU	CD	-24.19	-37.76	54.22	15.00
115	GLU	OE1	-23.20	-37.34	54.86	15.00
115	GLU	OE2	-24.10	-38.51	53.22	15.00
115	GLU	C	-28.52	-38.00	55.14	15.00
115	GLU	O	-28.72	-39.05	54.56	15.00
116	GLY	N	-29.21	-36.89	54.90	15.00
116	GLY	CA	-30.18	-36.81	53.83	15.00
116	GLY	C	-31.55	-37.41	54.07	15.00
116	GLY	O	-32.34	-37.53	53.14	15.00
117	ASN	N	-31.86	-37.73	55.32	15.00
117	ASN	CA	-33.15	-38.34	55.65	15.00
117	ASN	CB	-32.91	-39.54	56.56	15.00
117	ASN	CG	-34.17	-40.32	56.84	15.00
117	ASN	OD1	-35.26	-39.75	56.98	15.00
117	ASN	ND2	-34.04	-41.64	56.94	15.00
117	ASN	C	-34.11	-37.34	56.30	15.00
117	ASN	O	-34.16	-37.23	57.52	15.00
118	GLU	N	-34.90	-36.66	55.48	15.00
118	GLU	CA	-35.85	-35.67	55.98	15.00
118	GLU	CB	-36.67	-35.08	54.85	15.00
118	GLU	CG	-35.91	-34.08	54.01	15.00
118	GLU	CD	-36.80	-32.98	53.50	15.00
118	GLU	OE1	-37.51	-32.38	54.32	15.00
118	GLU	OE2	-36.79	-32.73	52.29	15.00
118	GLU	C	-36.80	-36.20	57.04	15.00

TABLE VI

118 GLU O	-37.05	-35.54	58.04	15.00
119 LYS N	-37.34	-37.38	56.81	15.00
119 LYS CA	-38.28	-37.95	57.77	15.00
119 LYS CB	-38.87	-39.24	57.21	15.00
119 LYS CG	-39.46	-39.06	55.80	15.00
119 LYS CD	-40.57	-38.01	55.77	15.00
119 LYS CE	-41.82	-38.49	56.49	15.00
119 LYS NZ	-42.97	-37.55	56.32	15.00
119 LYS C	-37.66	-38.15	59.15	15.00
119 LYS O	-38.29	-37.87	60.16	15.00
120 ALA N	-36.39	-38.56	59.19	15.00
120 ALA CA	-35.73	-38.76	60.48	15.00
120 ALA CB	-34.39	-39.43	60.30	15.00
120 ALA C	-35.56	-37.41	61.15	15.00
120 ALA O	-35.40	-37.34	62.37	15.00
121 LEU N	-35.58	-36.35	60.34	15.00
121 LEU CA	-35.45	-34.99	60.83	15.00
121 LEU CB	-35.03	-34.03	59.71	15.00
121 LEU CG	-34.92	-32.51	59.96	15.00
121 LEU CD1	-33.98	-32.21	61.11	15.00
121 LEU CD2	-34.45	-31.82	58.71	15.00
121 LEU C	-36.78	-34.54	61.43	15.00
121 LEU O	-36.80	-33.96	62.51	15.00
122 LYS N	-37.89	-34.84	60.76	15.00
122 LYS CA	-39.20	-34.44	61.28	15.00
122 LYS CB	-40.34	-34.86	60.35	15.00
122 LYS CG	-41.71	-34.49	60.95	15.00
122 LYS CD	-42.90	-34.72	60.02	15.00
122 LYS CE	-43.21	-36.19	59.84	15.00
122 LYS NZ	-42.13	-36.87	59.07	15.00
122 LYS C	-39.43	-35.03	62.67	15.00
122 LYS O	-40.00	-34.38	63.54	15.00
123 ARG N	-39.02	-36.28	62.85	15.00
123 ARG CA	-39.18	-36.96	64.12	15.00
123 ARG CB	-38.90	-38.45	63.95	15.00
123 ARG CG	-40.04	-39.22	63.30	15.00
123 ARG CD	-39.53	-40.52	62.67	15.00
123 ARG NE	-38.42	-41.08	63.44	15.00
123 ARG CZ	-37.46	-41.85	62.92	15.00
123 ARG NH1	-37.47	-42.16	61.62	15.00
123 ARG NH2	-36.45	-42.23	63.68	15.00
123 ARG C	-38.24	-36.34	65.14	15.00
123 ARG O	-38.65	-36.04	66.25	15.00

TABLE VI

124 ALA N	-36.99	-36.12	64.76	15.00
124 ALA CA	-36.05	-35.51	65.68	15.00
124 ALA CB	-34.70	-35.31	65.02	15.00
124 ALA C	-36.60	-34.17	66.19	15.00
124 ALA O	-36.55	-33.91	67.39	15.00
125 VAL N	-37.14	-33.34	65.30	15.00
125 VAL CA	-37.68	-32.06	65.76	15.00
125 VAL CB	-38.01	-31.03	64.60	15.00
125 VAL CG1	-36.78	-30.27	64.19	15.00
125 VAL CG2	-38.58	-31.72	63.39	15.00
125 VAL C	-38.94	-32.28	66.58	15.00
125 VAL O	-39.21	-31.52	67.50	15.00
126 ALA N	-39.69	-33.32	66.27	15.00
126 ALA CA	-40.93	-33.60	66.98	15.00
126 ALA CB	-41.81	-34.52	66.16	15.00
126 ALA C	-40.75	-34.16	68.38	15.00
126 ALA O	-41.53	-33.84	69.28	15.00
127 ARG N	-39.73	-35.00	68.55	15.00
127 ARG CA	-39.42	-35.68	69.81	15.00
127 ARG CB	-39.04	-37.14	69.54	15.00
127 ARG CG	-40.20	-37.95	69.00	15.00
127 ARG CD	-39.78	-39.23	68.27	15.00
127 ARG NE	-40.95	-39.80	67.60	15.00
127 ARG CZ	-40.95	-40.88	66.83	15.00
127 ARG NH1	-42.09	-41.30	66.28	15.00
127 ARG NH2	-39.84	-41.56	66.63	15.00
127 ARG C	-38.33	-35.04	70.66	15.00
127 ARG O	-38.25	-35.30	71.86	15.00
128 VAL N	-37.48	-34.22	70.04	15.00
128 VAL CA	-36.40	-33.54	70.75	15.00
128 VAL CB	-35.03	-33.81	70.10	15.00
128 VAL CG1	-33.92	-33.34	71.02	15.00
128 VAL CG2	-34.87	-35.29	69.78	15.00
128 VAL C	-36.58	-32.02	70.88	15.00
128 VAL O	-36.43	-31.46	71.95	15.00
129 GLY N	-36.89	-31.35	69.77	15.00
129 GLY CA	-37.08	-29.91	69.81	15.00
129 GLY C	-36.26	-29.29	68.69	15.00
129 GLY O	-36.02	-29.96	67.68	15.00
130 PRO N	-35.83	-28.02	68.81	15.00
130 PRO CD	-36.20	-27.06	69.86	15.00
130 PRO CA	-35.04	-27.37	67.77	15.00
130 PRO CB	-34.67	-26.05	68.43	15.00

TABLE VI

130 PRO CG	-35.92	-25.74	69.18	15.00
130 PRO C	-33.81	-28.17	67.39	15.00
130 PRO O	-33.07	-28.64	68.26	15.00
131 VAL N	-33.60	-28.33	66.09	15.00
131 VAL CA	-32.46	-29.08	65.58	15.00
131 VAL CB	-32.94	-30.26	64.68	15.00
131 VAL CG1	-31.76	-31.03	64.14	15.00
131 VAL CG2	-33.82	-31.20	65.46	15.00
131 VAL C	-31.50	-28.20	64.77	15.00
131 VAL O	-31.93	-27.35	63.99	15.00
132 SER N	-30.20	-28.39	64.96	15.00
132 SER CA	-29.23	-27.61	64.22	15.00
132 SER CB	-27.88	-27.61	64.94	15.00
132 SER OG	-28.00	-26.96	66.20	15.00
132 SER C	-29.08	-28.21	62.82	15.00
132 SER O	-28.83	-29.41	62.68	15.00
133 VAL N	-29.31	-27.39	61.80	15.00
133 VAL CA	-29.22	-27.82	60.40	15.00
133 VAL CB	-30.60	-27.81	59.68	15.00
133 VAL CG1	-31.51	-28.90	60.23	15.00
133 VAL CG2	-31.27	-26.45	59.80	15.00
133 VAL C	-28.26	-26.93	59.62	15.00
133 VAL O	-27.88	-25.85	60.08	15.00
134 ALA N	-27.93	-27.36	58.41	15.00
134 ALA CA	-27.02	-26.64	57.54	15.00
134 ALA CB	-25.69	-27.35	57.48	15.00
134 ALA C	-27.64	-26.61	56.16	15.00
134 ALA O	-27.92	-27.66	55.60	15.00
135 ILE N	-27.84	-25.43	55.60	15.00
135 ILE CA	-28.45	-25.31	54.28	15.00
135 ILE CB	-29.84	-24.62	54.36	15.00
135 ILE CG2	-30.82	-25.47	55.15	15.00
135 ILE CG1	-29.70	-23.24	55.00	15.00
135 ILE CD1	-30.95	-22.42	54.97	15.00
135 ILE C	-27.59	-24.49	53.32	15.00
135 ILE O	-26.49	-24.04	53.66	15.00
136 ASP N	-28.09	-24.33	52.10	15.00
136 ASP CA	-27.45	-23.52	51.07	15.00
136 ASP CB	-27.50	-24.23	49.72	15.00
136 ASP CG	-27.09	-23.32	48.57	15.00
136 ASP OD1	-27.71	-23.40	47.49	15.00
136 ASP OD2	-26.15	-22.50	48.73	15.00
136 ASP C	-28.22	-22.21	50.99	15.00

TABLE VI

136 ASP O	-29.36	-22.17	50.52	15.00
137 ALA N	-27.61	-21.13	51.46	15.00
137 ALA CA	-28.26	-19.83	51.42	15.00
137 ALA CB	-28.42	-19.30	52.83	15.00
137 ALA C	-27.46	-18.84	50.56	15.00
137 ALA O	-27.34	-17.66	50.89	15.00
138 SER N	-26.92	-19.34	49.45	15.00
138 SER CA	-26.12	-18.53	48.53	15.00
138 SER CB	-25.09	-19.42	47.83	15.00
138 SER OG	-25.71	-20.52	47.19	15.00
138 SER C	-26.97	-17.80	47.49	15.00
138 SER O	-26.60	-16.72	47.01	15.00
139 LEU N	-28.12	-18.36	47.17	15.00
139 LEU CA	-29.02	-17.79	46.19	15.00
139 LEU CB	-30.07	-18.84	45.80	15.00
139 LEU CG	-29.49	-20.25	45.62	15.00
139 LEU CD1	-30.58	-21.21	45.21	15.00
139 LEU CD2	-28.37	-20.28	44.61	15.00
139 LEU C	-29.70	-16.52	46.70	15.00
139 LEU O	-30.06	-16.43	47.88	15.00
140 THR N	-29.90	-15.54	45.81	15.00
140 THR CA	-30.54	-14.29	46.18	15.00
140 THR CB	-30.46	-13.21	45.07	15.00
140 THR OG1	-30.85	-13.77	43.82	15.00
140 THR CG2	-29.05	-12.66	44.96	15.00
140 THR C	-32.00	-14.49	46.57	15.00
140 THR O	-32.50	-13.79	47.45	15.00
141 SER N	-32.68	-15.45	45.95	15.00
141 SER CA	-34.08	-15.70	46.30	15.00
141 SER CB	-34.66	-16.86	45.50	15.00
141 SER OG	-33.72	-17.92	45.39	15.00
141 SER C	-34.19	-15.94	47.79	15.00
141 SER O	-35.04	-15.37	48.46	15.00
142 PHE N	-33.27	-16.72	48.33	15.00
142 PHE CA	-33.28	-17.01	49.76	15.00
142 PHE CB	-32.21	-18.05	50.11	15.00
142 PHE CG	-32.17	-18.41	51.57	15.00
142 PHE CD1	-32.97	-19.43	52.08	15.00
142 PHE CD2	-31.34	-17.72	52.45	15.00
142 PHE CE1	-32.94	-19.75	53.43	15.00
142 PHE CE2	-31.31	-18.04	53.80	15.00
142 PHE CZ	-32.11	-19.05	54.29	15.00
142 PHE C	-33.01	-15.75	50.54	15.00

TABLE VI

142 PHE O	-33.69	-15.45	51.52	15.00
143 GLN N	-32.01	-15.00	50.09	15.00
143 GLN CA	-31.61	-13.79	50.78	15.00
143 GLN CB	-30.30	-13.26	50.21	15.00
143 GLN CG	-29.18	-14.29	50.23	15.00
143 GLN CD	-27.85	-13.72	49.81	15.00
143 GLN OE1	-27.29	-12.84	50.48	15.00
143 GLN NE2	-27.31	-14.22	48.70	15.00
143 GLN C	-32.67	-12.70	50.84	15.00
143 GLN O	-32.79	-12.04	51.86	15.00
144 PHE N	-33.45	-12.51	49.78	15.00
144 PHE CA	-34.50	-11.48	49.83	15.00
144 PHE CB	-34.57	-10.60	48.55	15.00
144 PHE CG	-34.78	-11.35	47.27	15.00
144 PHE CD1	-33.92	-11.14	46.19	15.00
144 PHE CD2	-35.84	-12.24	47.12	15.00
144 PHE CE1	-34.11	-11.81	44.99	15.00
144 PHE CE2	-36.04	-12.92	45.91	15.00
144 PHE CZ	-35.18	-12.71	44.85	15.00
144 PHE C	-35.88	-12.04	50.20	15.00
144 PHE O	-36.90	-11.36	50.02	15.00
145 TYR N	-35.89	-13.28	50.71	15.00
145 TYR CA	-37.12	-13.95	51.12	15.00
145 TYR CB	-36.80	-15.21	51.94	15.00
145 TYR CG	-37.98	-15.77	52.70	15.00
145 TYR CD1	-38.84	-16.69	52.12	15.00
145 TYR CE1	-39.96	-17.15	52.80	15.00
145 TYR CD2	-38.27	-15.32	53.99	15.00
145 TYR CE2	-39.40	-15.78	54.67	15.00
145 TYR CZ	-40.24	-16.69	54.07	15.00
145 TYR OH	-41.38	-17.11	54.73	15.00
145 TYR C	-37.90	-12.98	51.97	15.00
145 TYR O	-37.32	-12.24	52.74	15.00
146 SER N	-39.21	-13.02	51.84	15.00
146 SER CA	-40.07	-12.13	52.59	15.00
146 SER CB	-40.63	-11.07	51.63	15.00
146 SER OG	-41.38	-10.08	52.30	15.00
146 SER C	-41.21	-12.89	53.24	15.00
146 SER O	-41.48	-12.72	54.43	15.00
147 LYS N	-41.86	-13.77	52.48	15.00
147 LYS CA	-42.98	-14.54	53.01	15.00
147 LYS CB	-44.25	-13.71	53.04	15.00
147 LYS CG	-44.62	-13.11	51.70	15.00

TABLE VI

147 LYS CD	-46.07	-12.67	51.68	15.00
147 LYS CE	-46.47	-12.13	50.31	15.00
147 LYS NZ	-47.97	-12.11	50.14	15.00
147 LYS C	-43.21	-15.79	52.19	15.00
147 LYS O	-42.55	-16.01	51.17	15.00
148 GLY N	-44.16	-16.61	52.64	15.00
148 GLY CA	-44.49	-17.85	51.95	15.00
148 GLY C	-43.47	-18.95	52.16	15.00
148 GLY O	-42.52	-18.79	52.93	15.00
149 VAL N	-43.64	-20.04	51.43	15.00
149 VAL CA	-42.75	-21.19	51.52	15.00
149 VAL CB	-43.57	-22.51	51.47	15.00
149 VAL CG1	-42.66	-23.71	51.33	15.00
149 VAL CG2	-44.41	-22.65	52.72	15.00
149 VAL C	-41.67	-21.17	50.43	15.00
149 VAL O	-41.96	-21.34	49.24	15.00
150 TYR N	-40.43	-20.96	50.84	15.00
150 TYR CA	-39.30	-20.91	49.91	15.00
150 TYR CB	-38.04	-20.41	50.64	15.00
150 TYR CG	-36.82	-20.29	49.75	15.00
150 TYR CD1	-36.78	-19.38	48.69	15.00
150 TYR CE1	-35.67	-19.27	47.88	15.00
150 TYR CD2	-35.69	-21.07	49.97	15.00
150 TYR CE2	-34.56	-20.96	49.16	15.00
150 TYR CZ	-34.56	-20.06	48.11	15.00
150 TYR OH	-33.45	-19.93	47.32	15.00
150 TYR C	-39.03	-22.26	49.27	15.00
150 TYR O	-39.23	-23.31	49.88	15.00
151 TYR N	-38.55	-22.22	48.03	15.00
151 TYR CA	-38.21	-23.42	47.28	15.00
151 TYR CB	-39.45	-24.26	46.99	15.00
151 TYR CG	-39.15	-25.46	46.11	15.00
151 TYR CD1	-38.22	-26.42	46.51	15.00
151 TYR CE1	-37.94	-27.53	45.71	15.00
151 TYR CD2	-39.79	-25.63	44.89	15.00
151 TYR CE2	-39.52	-26.74	44.08	15.00
151 TYR CZ	-38.59	-27.69	44.50	15.00
151 TYR OH	-38.36	-28.83	43.75	15.00
151 TYR C	-37.60	-23.00	45.97	15.00
151 TYR O	-38.29	-22.44	45.11	15.00
152 ASP N	-36.31	-23.25	45.80	15.00
152 ASP CA	-35.66	-22.90	44.55	15.00
152 ASP CB	-34.74	-21.69	44.71	15.00

TABLE VI

152 ASP CG	-34.02	-21.34	43.43	15.00
152 ASP OD1	-34.60	-21.55	42.34	15.00
152 ASP OD2	-32.87	-20.86	43.49	15.00
152 ASP C	-34.87	-24.07	44.02	15.00
152 ASP O	-33.84	-24.43	44.56	15.00
153 GLU N	-35.33	-24.60	42.90	15.00
153 GLU CA	-34.70	-25.74	42.26	15.00
153 GLU CB	-35.49	-26.18	41.03	15.00
153 GLU CG	-35.79	-25.08	40.01	15.00
153 GLU CD	-37.17	-24.43	40.19	15.00
153 GLU OE1	-38.12	-24.84	39.48	15.00
153 GLU OE2	-37.29	-23.50	41.02	15.00
153 GLU C	-33.22	-25.56	41.91	15.00
153 GLU O	-32.59	-26.50	41.44	15.00
154 SER N	-32.66	-24.37	42.12	15.00
154 SER CA	-31.24	-24.12	41.82	15.00
154 SER CB	-31.02	-22.70	41.29	15.00
154 SER OG	-32.05	-22.32	40.40	15.00
154 SER C	-30.40	-24.30	43.08	15.00
154 SER O	-29.17	-24.21	43.04	15.00
155 CYS N	-31.08	-24.48	44.22	15.00
155 CYS CA	-30.41	-24.66	45.49	15.00
155 CYS C	-29.57	-25.91	45.40	15.00
155 CYS O	-30.00	-26.91	44.82	15.00
155 CYS CB	-31.44	-24.79	46.62	15.00
155 CYS SG	-30.90	-24.05	48.19	15.00
156 ASN N	-28.36	-25.87	45.94	15.00
156 ASN CA	-27.47	-27.01	45.87	15.00
156 ASN CB	-26.18	-26.59	45.19	15.00
156 ASN CG	-25.28	-27.76	44.91	15.00
156 ASN OD1	-25.73	-28.91	44.88	15.00
156 ASN ND2	-23.99	-27.49	44.73	15.00
156 ASN C	-27.20	-27.67	47.23	15.00
156 ASN O	-26.43	-27.16	48.05	15.00
157 SER N	-27.79	-28.85	47.41	15.00
157 SER CA	-27.67	-29.64	48.62	15.00
157 SER CB	-28.48	-30.92	48.45	15.00
157 SER OG	-29.83	-30.63	48.13	15.00
157 SER C	-26.24	-30.00	49.04	15.00
157 SER O	-26.01	-30.36	50.19	15.00
158 ASP N	-25.30	-29.93	48.10	15.00
158 ASP CA	-23.89	-30.24	48.35	15.00
158 ASP CB	-23.21	-30.69	47.07	15.00

TABLE VI

158 ASP CG	-23.72	-32.01	46.57	15.00
158 ASP OD1	-24.95	-32.15	46.33	15.00
158 ASP OD2	-22.86	-32.91	46.38	15.00
158 ASP C	-23.14	-29.02	48.87	15.00
158 ASP O	-22.11	-29.15	49.53	15.00
159 ASN N	-23.62	-27.84	48.51	15.00
159 ASN CA	-22.98	-26.62	48.94	15.00
159 ASN CB	-23.10	-25.57	47.84	15.00
159 ASN CG	-22.14	-24.40	48.03	15.00
159 ASN OD1	-21.43	-24.30	49.04	15.00
159 ASN ND2	-22.10	-23.51	47.04	15.00
159 ASN C	-23.68	-26.14	50.20	15.00
159 ASN O	-24.63	-25.37	50.12	15.00
160 LEU N	-23.25	-26.64	51.36	15.00
160 LEU CA	-23.84	-26.23	52.63	15.00
160 LEU CB	-23.88	-27.42	53.60	15.00
160 LEU CG	-24.59	-28.72	53.22	15.00
160 LEU CD1	-24.45	-29.70	54.37	15.00
160 LEU CD2	-26.06	-28.49	52.89	15.00
160 LEU C	-22.98	-25.11	53.22	15.00
160 LEU O	-21.91	-25.35	53.78	15.00
161 ASN N	-23.47	-23.89	53.16	15.00
161 ASN CA	-22.70	-22.75	53.65	15.00
161 ASN CB	-22.58	-21.73	52.53	15.00
161 ASN CG	-23.89	-21.51	51.84	15.00
161 ASN OD1	-24.74	-20.76	52.33	15.00
161 ASN ND2	-24.10	-22.23	50.75	15.00
161 ASN C	-23.23	-22.05	54.89	15.00
161 ASN O	-22.45	-21.62	55.73	15.00
162 HIS N	-24.54	-21.93	55.01	15.00
162 HIS CA	-25.13	-21.27	56.16	15.00
162 HIS CB	-26.18	-20.27	55.67	15.00
162 HIS CG	-26.55	-19.22	56.67	15.00
162 HIS CD2	-27.72	-18.61	56.93	15.00
162 HIS ND1	-25.63	-18.66	57.53	15.00
162 HIS CE1	-26.22	-17.74	58.27	15.00
162 HIS NE2	-27.49	-17.69	57.93	15.00
162 HIS C	-25.76	-22.27	57.12	15.00
162 HIS O	-26.47	-23.19	56.69	15.00
163 ALA N	-25.47	-22.12	58.41	15.00
163 ALA CA	-26.01	-23.00	59.45	15.00
163 ALA CB	-24.93	-23.33	60.47	15.00
163 ALA C	-27.15	-22.28	60.13	15.00

TABLE VI

163 ALA O	-27.00	-21.13	60.54	15.00
164 VAL N	-28.30	-22.94	60.24	15.00
164 VAL CA	-29.48	-22.34	60.86	15.00
164 VAL CB	-30.54	-21.99	59.79	15.00
164 VAL CG1	-30.11	-20.79	58.99	15.00
164 VAL CG2	-30.75	-23.16	58.86	15.00
164 VAL C	-30.05	-23.28	61.91	15.00
164 VAL O	-29.37	-24.21	62.33	15.00
165 LEU N	-31.31	-23.07	62.30	15.00
165 LEU CA	-31.97	-23.88	63.33	15.00
165 LEU CB	-32.00	-23.11	64.64	15.00
165 LEU CG	-32.59	-23.77	65.88	15.00
165 LEU CD1	-31.53	-24.65	66.49	15.00
165 LEU CD2	-33.04	-22.71	66.87	15.00
165 LEU C	-33.40	-24.17	62.94	15.00
165 LEU O	-34.16	-23.24	62.72	15.00
166 ALA N	-33.79	-25.44	62.92	15.00
166 ALA CA	-35.15	-25.82	62.56	15.00
166 ALA CB	-35.16	-27.19	61.92	15.00
166 ALA C	-36.03	-25.80	63.80	15.00
166 ALA O	-35.93	-26.66	64.66	15.00
167 VAL N	-36.89	-24.80	63.88	15.00
167 VAL CA	-37.79	-24.62	65.01	15.00
167 VAL CB	-38.11	-23.11	65.18	15.00
167 VAL CG1	-39.35	-22.88	66.00	15.00
167 VAL CG2	-36.94	-22.42	65.84	15.00
167 VAL C	-39.06	-25.46	64.92	15.00
167 VAL O	-39.83	-25.56	65.87	15.00
168 GLY N	-39.28	-26.10	63.78	15.00
168 GLY CA	-40.48	-26.91	63.65	15.00
168 GLY C	-40.77	-27.29	62.23	15.00
168 GLY O	-39.85	-27.36	61.41	15.00
169 TYR N	-42.04	-27.55	61.95	15.00
169 TYR CA	-42.50	-27.93	60.62	15.00
169 TYR CB	-42.09	-29.38	60.30	15.00
169 TYR CG	-42.61	-30.41	61.28	15.00
169 TYR CD1	-43.94	-30.82	61.25	15.00
169 TYR CE1	-44.42	-31.76	62.13	15.00
169 TYR CD2	-41.77	-30.98	62.23	15.00
169 TYR CE2	-42.24	-31.93	63.13	15.00
169 TYR CZ	-43.57	-32.31	63.07	15.00
169 TYR OH	-44.04	-33.26	63.95	15.00
169 TYR C	-44.02	-27.78	60.54	15.00

TABLE VI

169 TYR O	-44.70	-27.74	61.57	15.00
170 GLY N	-44.55	-27.71	59.33	15.00
170 GLY CA	-45.98	-27.55	59.16	15.00
170 GLY C	-46.42	-27.49	57.72	15.00
170 GLY O	-45.69	-27.89	56.82	15.00
171 ILE N	-47.61	-26.95	57.49	15.00
171 ILE CA	-48.20	-26.83	56.16	15.00
171 ILE CB	-49.51	-27.69	56.06	15.00
171 ILE CG2	-50.16	-27.55	54.70	15.00
171 ILE CG1	-49.20	-29.18	56.27	15.00
171 ILE CD1	-48.97	-29.59	57.73	15.00
171 ILE C	-48.55	-25.36	55.90	15.00
171 ILE O	-48.58	-24.55	56.84	15.00
172 GLN N	-48.73	-25.00	54.63	15.00
172 GLN CA	-49.10	-23.64	54.25	15.00
172 GLN CB	-47.90	-22.90	53.68	15.00
172 GLN CG	-47.16	-22.04	54.69	15.00
172 GLN CD	-47.81	-20.68	54.87	15.00
172 GLN OE1	-47.24	-19.66	54.49	15.00
172 GLN NE2	-49.00	-20.66	55.47	15.00
172 GLN C	-50.24	-23.71	53.24	15.00
172 GLN O	-51.31	-24.23	53.55	15.00
173 LYS N	-50.05	-23.17	52.05	15.00
173 LYS CA	-51.11	-23.24	51.05	15.00
173 LYS CB	-51.04	-22.05	50.08	15.00
173 LYS CG	-51.15	-20.70	50.77	15.00
173 LYS CD	-50.94	-19.57	49.77	15.00
173 LYS CE	-50.57	-18.27	50.50	15.00
173 LYS NZ	-49.28	-18.39	51.26	15.00
173 LYS C	-50.82	-24.55	50.34	15.00
173 LYS O	-50.33	-24.58	49.21	15.00
174 GLY N	-51.02	-25.63	51.08	15.00
174 GLY CA	-50.77	-26.96	50.56	15.00
174 GLY C	-49.30	-27.32	50.59	15.00
174 GLY O	-48.95	-28.47	50.31	15.00
175 ASN N	-48.44	-26.35	50.92	15.00
175 ASN CA	-47.00	-26.60	50.98	15.00
175 ASN CB	-46.20	-25.39	50.47	15.00
175 ASN CG	-46.70	-24.86	49.14	15.00
175 ASN OD1	-47.33	-23.79	49.08	15.00
175 ASN ND2	-46.41	-25.58	48.06	15.00
175 ASN C	-46.49	-26.95	52.38	15.00
175 ASN O	-46.66	-26.16	53.33	15.00

TABLE VI

176 LYS N	-45.90	-28.13	52.53	15.00
176 LYS CA	-45.33	-28.50	53.82	15.00
176 LYS CB	-44.94	-29.98	53.84	15.00
176 LYS CG	-46.10	-30.95	53.63	15.00
176 LYS CD	-45.67	-32.36	53.98	15.00
176 LYS CE	-46.71	-33.40	53.61	15.00
176 LYS NZ	-46.36	-34.11	52.34	15.00
176 LYS C	-44.08	-27.63	53.94	15.00
176 LYS O	-43.52	-27.21	52.92	15.00
177 HIS N	-43.62	-27.37	55.16	15.00
177 HIS CA	-42.44	-26.52	55.34	15.00
177 HIS CB	-42.84	-25.05	55.23	15.00
177 HIS CG	-43.71	-24.59	56.35	15.00
177 HIS CD2	-43.41	-24.18	57.61	15.00
177 HIS ND1	-45.09	-24.52	56.26	15.00
177 HIS CE1	-45.59	-24.10	57.40	15.00
177 HIS NE2	-44.59	-23.89	58.24	15.00
177 HIS C	-41.74	-26.73	56.67	15.00
177 HIS O	-42.32	-27.24	57.62	15.00
178 TRP N	-40.49	-26.28	56.73	15.00
178 TRP CA	-39.64	-26.34	57.91	15.00
178 TRP CB	-38.24	-26.82	57.54	15.00
178 TRP CG	-38.16	-28.22	57.08	15.00
178 TRP CD2	-38.28	-29.41	57.88	15.00
178 TRP CE2	-38.08	-30.51	57.03	15.00
178 TRP CE3	-38.52	-29.64	59.24	15.00
178 TRP CD1	-37.92	-28.65	55.81	15.00
178 TRP NE1	-37.87	-30.02	55.77	15.00
178 TRP CZ2	-38.13	-31.83	57.48	15.00
178 TRP CZ3	-38.57	-30.95	59.70	15.00
178 TRP CH2	-38.37	-32.03	58.83	15.00
178 TRP C	-39.53	-24.91	58.39	15.00
178 TRP O	-39.15	-24.04	57.61	15.00
179 ILE N	-39.89	-24.63	59.63	15.00
179 ILE CA	-39.79	-23.28	60.16	15.00
179 ILE CB	-40.65	-23.09	61.42	15.00
179 ILE CG2	-40.61	-21.64	61.85	15.00
179 ILE CG1	-42.09	-23.52	61.15	15.00
179 ILE CD1	-42.97	-23.45	62.38	15.00
179 ILE C	-38.32	-23.04	60.52	15.00
179 ILE O	-37.80	-23.66	61.45	15.00
180 ILE N	-37.67	-22.16	59.78	15.00
180 ILE CA	-36.27	-21.87	60.01	15.00

TABLE VI

180 ILE CB	-35.46	-22.00	58.70	15.00
180 ILE CG2	-34.01	-21.64	58.91	15.00
180 ILE CG1	-35.57	-23.42	58.16	15.00
180 ILE CD1	-34.96	-24.46	59.08	15.00
180 ILE C	-36.01	-20.52	60.69	15.00
180 ILE O	-36.70	-19.53	60.44	15.00
181 LYS N	-35.02	-20.53	61.58	15.00
181 LYS CA	-34.60	-19.36	62.34	15.00
181 LYS CB	-34.59	-19.69	63.84	15.00
181 LYS CG	-34.02	-18.59	64.70	15.00
181 LYS CD	-33.87	-19.04	66.14	15.00
181 LYS CE	-33.58	-17.85	67.01	15.00
181 LYS NZ	-33.52	-18.17	68.45	15.00
181 LYS C	-33.19	-19.02	61.91	15.00
181 LYS O	-32.28	-19.85	62.04	15.00
182 ASN N	-33.00	-17.82	61.37	15.00
182 ASN CA	-31.68	-17.42	60.93	15.00
182 ASN CB	-31.77	-16.80	59.54	15.00
182 ASN CG	-30.45	-16.80	58.83	15.00
182 ASN OD1	-29.40	-16.99	59.44	15.00
182 ASN ND2	-30.48	-16.62	57.51	15.00
182 ASN C	-31.10	-16.42	61.92	15.00
182 ASN O	-31.81	-15.94	62.79	15.00
183 SER N	-29.81	-16.14	61.82	15.00
183 SER CA	-29.19	-15.20	62.74	15.00
183 SER CB	-27.97	-15.85	63.38	15.00
183 SER OG	-27.30	-16.66	62.44	15.00
183 SER C	-28.79	-13.90	62.04	15.00
183 SER O	-27.68	-13.40	62.23	15.00
184 TRP N	-29.70	-13.34	61.25	15.00
184 TRP CA	-29.44	-12.11	60.52	15.00
184 TRP CB	-29.77	-12.29	59.03	15.00
184 TRP CG	-28.79	-13.14	58.29	15.00
184 TRP CD2	-28.97	-13.73	57.01	15.00
184 TRP CE2	-27.80	-14.45	56.71	15.00
184 TRP CE3	-30.01	-13.74	56.08	15.00
184 TRP CD1	-27.55	-13.50	58.71	15.00
184 TRP NE1	-26.94	-14.28	57.77	15.00
184 TRP CZ2	-27.64	-15.17	55.52	15.00
184 TRP CZ3	-29.85	-14.46	54.90	15.00
184 TRP CH2	-28.67	-15.16	54.63	15.00
184 TRP C	-30.23	-10.93	61.07	15.00
184 TRP O	-30.32	-9.88	60.43	15.00

TABLE VI

185 GLY N	-30.78	-11.07	62.27	15.00
185 GLY CA	-31.54	-9.98	62.83	15.00
185 GLY C	-33.02	-10.16	62.62	15.00
185 GLY O	-33.46	-11.00	61.84	15.00
186 GLU N	-33.80	-9.35	63.33	15.00
186 GLU CA	-35.26	-9.39	63.27	15.00
186 GLU CB	-35.79	-8.71	64.53	15.00
186 GLU CG	-37.29	-8.65	64.70	15.00
186 GLU CD	-37.71	-8.03	66.04	15.00
186 GLU OE1	-36.83	-7.61	66.83	15.00
186 GLU OE2	-38.93	-7.98	66.31	15.00
186 GLU C	-35.73	-8.65	62.03	15.00
186 GLU O	-36.89	-8.73	61.64	15.00
187 ASN N	-34.78	-8.02	61.36	15.00
187 ASN CA	-35.02	-7.21	60.18	15.00
187 ASN CB	-34.03	-6.03	60.25	15.00
187 ASN CG	-34.42	-4.86	59.37	15.00
187 ASN OD1	-33.58	-4.33	58.64	15.00
187 ASN ND2	-35.67	-4.40	59.48	15.00
187 ASN C	-34.86	-7.97	58.86	15.00
187 ASN O	-34.92	-7.36	57.80	15.00
188 TRP N	-34.62	-9.28	58.92	15.00
188 TRP CA	-34.47	-10.08	57.70	15.00
188 TRP CB	-33.20	-10.94	57.77	15.00
188 TRP CG	-33.05	-11.85	56.60	15.00
188 TRP CD2	-33.41	-13.23	56.52	15.00
188 TRP CE2	-33.18	-13.66	55.20	15.00
188 TRP CE3	-33.92	-14.16	57.45	15.00
188 TRP CD1	-32.61	-11.50	55.36	15.00
188 TRP NE1	-32.69	-12.58	54.51	15.00
188 TRP CZ2	-33.45	-14.96	54.76	15.00
188 TRP CZ3	-34.18	-15.46	57.02	15.00
188 TRP CH2	-33.94	-15.85	55.69	15.00
188 TRP C	-35.66	-11.00	57.51	15.00
188 TRP O	-36.23	-11.48	58.49	15.00
189 GLY N	-36.02	-11.29	56.27	15.00
189 GLY CA	-37.14	-12.17	56.00	15.00
189 GLY C	-38.37	-11.86	56.84	15.00
189 GLY O	-38.70	-10.69	57.08	15.00
190 ASN N	-39.02	-12.91	57.32	15.00
190 ASN CA	-40.22	-12.78	58.13	15.00
190 ASN CB	-41.13	-14.00	57.93	15.00
190 ASN CG	-42.58	-13.74	58.32	15.00

TABLE VI

190 ASN OD1	-42.87	-13.07	59.31	15.00
190 ASN ND2	-43.50	-14.27	57.53	15.00
190 ASN C	-39.86	-12.63	59.61	15.00
190 ASN O	-39.81	-13.61	60.35	15.00
191 LYS N	-39.55	-11.41	60.02	15.00
191 LYS CA	-39.19	-11.14	61.41	15.00
191 LYS CB	-40.43	-11.19	62.29	15.00
191 LYS CG	-41.44	-10.10	61.96	15.00
191 LYS CD	-40.92	-8.71	62.35	15.00
191 LYS CE	-41.18	-7.63	61.27	15.00
191 LYS NZ	-40.19	-7.69	60.13	15.00
191 LYS C	-38.10	-12.07	61.94	15.00
191 LYS O	-38.11	-12.46	63.11	15.00
192 GLY N	-37.15	-12.41	61.07	15.00
192 GLY CA	-36.04	-13.26	61.47	15.00
192 GLY C	-36.15	-14.73	61.13	15.00
192 GLY O	-35.19	-15.48	61.32	15.00
193 TYR N	-37.30	-15.16	60.63	15.00
193 TYR CA	-37.50	-16.56	60.28	15.00
193 TYR CB	-38.69	-17.14	61.04	15.00
193 TYR CG	-38.47	-17.29	62.51	15.00
193 TYR CD1	-38.57	-16.19	63.36	15.00
193 TYR CE1	-38.34	-16.32	64.72	15.00
193 TYR CD2	-38.13	-18.51	63.06	15.00
193 TYR CE2	-37.91	-18.65	64.42	15.00
193 TYR CZ	-38.01	-17.55	65.24	15.00
193 TYR OH	-37.78	-17.71	66.59	15.00
193 TYR C	-37.76	-16.73	58.80	15.00
193 TYR O	-37.97	-15.76	58.08	15.00
194 ILE N	-37.78	-17.99	58.37	15.00
194 ILE CA	-38.03	-18.32	56.99	15.00
194 ILE CB	-36.75	-18.27	56.13	15.00
194 ILE CG2	-35.65	-19.10	56.76	15.00
194 ILE CG1	-37.06	-18.74	54.72	15.00
194 ILE CD1	-35.95	-18.54	53.75	15.00
194 ILE C	-38.65	-19.70	56.88	15.00
194 ILE O	-38.20	-20.64	57.51	15.00
195 LEU N	-39.71	-19.79	56.09	15.00
195 LEU CA	-40.40	-21.04	55.87	15.00
195 LEU CB	-41.91	-20.78	55.71	15.00
195 LEU CG	-42.77	-20.89	56.98	15.00
195 LEU CD1	-42.08	-20.31	58.19	15.00
195 LEU CD2	-44.09	-20.19	56.75	15.00

TABLE VI

195 LEU C	-39.83	-21.68	54.62	15.00
195 LEU O	-40.04	-21.19	53.51	15.00
196 MET N	-39.05	-22.73	54.81	15.00
196 MET CA	-38.44	-23.44	53.70	15.00
196 MET CB	-37.01	-23.80	54.04	15.00
196 MET CG	-36.11	-22.58	54.16	15.00
196 MET SD	-34.46	-22.98	54.73	15.00
196 MET CE	-33.78	-23.75	53.28	15.00
196 MET C	-39.27	-24.68	53.38	15.00
196 MET O	-40.03	-25.14	54.23	15.00
197 ALA N	-39.15	-25.19	52.16	15.00
197 ALA CA	-39.91	-26.36	51.72	15.00
197 ALA CB	-39.86	-26.48	50.19	15.00
197 ALA C	-39.51	-27.69	52.36	15.00
197 ALA O	-38.33	-28.00	52.50	15.00
198 ARG N	-40.52	-28.50	52.67	15.00
198 ARG CA	-40.32	-29.81	53.28	15.00
198 ARG CB	-41.08	-29.90	54.60	15.00
198 ARG CG	-41.09	-31.28	55.23	15.00
198 ARG CD	-41.40	-31.21	56.71	15.00
198 ARG NE	-42.71	-30.64	57.00	15.00
198 ARG CZ	-43.83	-31.35	57.04	15.00
198 ARG NH1	-43.80	-32.66	56.80	15.00
198 ARG NH2	-44.97	-30.76	57.34	15.00
198 ARG C	-40.79	-30.90	52.34	15.00
198 ARG O	-41.87	-30.81	51.76	15.00
199 ASN N	-39.97	-31.93	52.20	15.00
199 ASN CA	-40.28	-33.07	51.33	15.00
199 ASN CB	-41.68	-33.62	51.60	15.00
199 ASN CG	-41.76	-34.41	52.90	15.00
199 ASN OD1	-42.80	-34.44	53.57	15.00
199 ASN ND2	-40.65	-35.05	53.28	15.00
199 ASN C	-40.08	-32.78	49.85	15.00
199 ASN O	-40.45	-33.59	48.99	15.00
200 LYS N	-39.47	-31.65	49.54	15.00
200 LYS CA	-39.18	-31.30	48.16	15.00
200 LYS CB	-39.18	-29.77	47.95	15.00
200 LYS CG	-40.55	-29.15	47.76	15.00
200 LYS CD	-41.24	-29.74	46.54	15.00
200 LYS CE	-42.64	-29.19	46.34	15.00
200 LYS NZ	-43.39	-29.98	45.32	15.00
200 LYS C	-37.80	-31.87	47.84	15.00
200 LYS O	-36.86	-31.13	47.56	15.00

TABLE VI

201 ASN N	-37.66	-33.19	48.01	15.00
201 ASN CA	-36.40	-33.87	47.72	15.00
201 ASN CB	-36.24	-33.99	46.19	15.00
201 ASN CG	-35.16	-35.00	45.77	15.00
201 ASN OD1	-35.27	-35.62	44.69	15.00
201 ASN ND2	-34.11	-35.15	46.58	15.00
201 ASN C	-35.18	-33.16	48.34	15.00
201 ASN O	-34.28	-32.70	47.62	15.00
202 ASN N	-35.16	-33.09	49.67	15.00
202 ASN CA	-34.05	-32.47	50.41	15.00
202 ASN CB	-32.86	-33.43	50.47	15.00
202 ASN CG	-31.99	-33.22	51.69	15.00
202 ASN OD1	-32.43	-32.60	52.67	15.00
202 ASN ND2	-30.77	-33.72	51.66	15.00
202 ASN C	-33.61	-31.11	49.86	15.00
202 ASN O	-32.42	-30.87	49.62	15.00
203 ALA N	-34.58	-30.22	49.72	15.00
203 ALA H	-35.43	-30.48	50.10	15.00
203 ALA CA	-34.36	-28.88	49.17	15.00
203 ALA CB	-35.62	-28.06	49.20	15.00
203 ALA C	-33.31	-28.14	50.00	15.00
203 ALA O	-33.47	-27.92	51.19	15.00
204 CYS N	-32.23	-27.75	49.33	15.00
204 CYS CA	-31.15	-27.01	49.98	15.00
204 CYS C	-30.39	-27.80	51.03	15.00
204 CYS O	-29.68	-27.21	51.83	15.00
204 CYS CB	-31.68	-25.71	50.61	15.00
204 CYS SG	-32.40	-24.49	49.47	15.00
205 GLY N	-30.51	-29.13	51.01	15.00
205 GLY CA	-29.80	-29.96	51.97	15.00
205 GLY C	-30.19	-29.78	53.44	15.00
205 GLY O	-29.39	-30.02	54.34	15.00
206 ILE N	-31.43	-29.40	53.67	15.00
206 ILE CA	-31.94	-29.18	55.01	15.00
206 ILE CB	-33.46	-28.88	54.98	15.00
206 ILE CG2	-34.18	-29.93	54.15	15.00
206 ILE CG1	-34.03	-28.79	56.39	15.00
206 ILE CD1	-33.55	-27.60	57.17	15.00
206 ILE C	-31.63	-30.32	55.98	15.00
206 ILE O	-31.31	-30.07	57.15	15.00
207 ALA N	-31.68	-31.56	55.50	15.00
207 ALA CA	-31.40	-32.72	56.36	15.00
207 ALA CB	-32.50	-33.74	56.24	15.00

TABLE VI

207 ALA C	-30.07	-33.37	56.02	15.00
207 ALA O	-29.89	-34.56	56.21	15.00
208 ASN N	-29.11	-32.58	55.55	15.00
208 ASN CA	-27.81	-33.10	55.16	15.00
208 ASN CB	-27.34	-32.39	53.88	15.00
208 ASN CG	-27.15	-33.35	52.72	15.00
208 ASN OD1	-28.12	-33.85	52.15	15.00
208 ASN ND2	-25.90	-33.60	52.36	15.00
208 ASN C	-26.72	-33.00	56.22	15.00
208 ASN O	-25.66	-33.62	56.10	15.00
209 LEU N	-26.96	-32.22	57.27	15.00
209 LEU CA	-25.96	-32.06	58.31	15.00
209 LEU CB	-24.98	-30.96	57.89	15.00
209 LEU CG	-23.69	-30.69	58.67	15.00
209 LEU CD1	-22.77	-31.90	58.61	15.00
209 LEU CD2	-22.99	-29.49	58.09	15.00
209 LEU C	-26.63	-31.70	59.63	15.00
209 LEU O	-26.11	-30.91	60.41	15.00
210 ALA N	-27.79	-32.31	59.90	15.00
210 ALA H	-28.15	-32.83	59.17	15.00
210 ALA CA	-28.56	-32.01	61.10	15.00
210 ALA CB	-29.98	-32.52	60.98	15.00
210 ALA C	-27.93	-32.71	62.32	15.00
210 ALA O	-27.23	-33.70	62.23	15.00
211 SER N	-28.20	-32.12	63.50	15.00
211 SER CA	-27.73	-32.66	64.78	15.00
211 SER CB	-26.21	-32.55	64.89	15.00
211 SER OG	-25.79	-31.20	64.98	15.00
211 SER C	-28.38	-31.89	65.92	15.00
211 SER O	-28.93	-30.80	65.72	15.00
212 PHE N	-28.35	-32.47	67.11	15.00
212 PHE CA	-28.93	-31.84	68.28	15.00
212 PHE CB	-30.43	-32.16	68.36	15.00
212 PHE CG	-30.75	-33.63	68.34	15.00
212 PHE CD1	-31.28	-34.23	67.20	15.00
212 PHE CD2	-30.55	-34.43	69.48	15.00
212 PHE CE1	-31.61	-35.57	67.19	15.00
212 PHE CE2	-30.87	-35.79	69.48	15.00
212 PHE CZ	-31.40	-36.35	68.33	15.00
212 PHE C	-28.17	-32.36	69.50	15.00
212 PHE O	-27.66	-33.48	69.48	15.00
213 PRO N	-28.03	-31.54	70.55	15.00
213 PRO CD	-28.53	-30.16	70.68	15.00

TABLE VI

213	PRO	CA	-27.32	-31.95	71.76	15.00
213	PRO	CB	-26.95	-30.61	72.38	15.00
213	PRO	CG	-28.16	-29.81	72.11	15.00
213	PRO	C	-28.20	-32.77	72.70	15.00
213	PRO	O	-29.42	-32.64	72.69	15.00
214	LYS	N	-27.58	-33.60	73.53	15.00
214	LYS	CA	-28.32	-34.41	74.49	15.00
214	LYS	CB	-27.85	-35.85	74.47	15.00
214	LYS	CG	-28.28	-36.60	73.23	15.00
214	LYS	CD	-27.98	-38.09	73.30	15.00
214	LYS	CE	-26.48	-38.39	73.31	15.00
214	LYS	NZ	-25.86	-38.24	74.66	15.00
214	LYS	C	-28.17	-33.84	75.89	15.00
214	LYS	O	-27.07	-33.47	76.29	15.00
215	MET	N	-29.28	-33.75	76.61	15.00
215	MET	CA	-29.29	-33.24	77.98	15.00
215	MET	CB	-30.27	-32.08	78.11	15.00
215	MET	CG	-29.79	-30.79	77.48	15.00
215	MET	SD	-28.97	-29.73	78.67	15.00
215	MET	CE	-30.38	-28.92	79.43	15.00
215	MET	C	-29.67	-34.33	78.99	15.00
215	MET	OT1	-30.25	-35.37	78.59	15.00
215	MET	OT2	-29.39	-34.13	80.20	15.00
216	HOH	OH2	-21.96	-40.63	81.12	15.00
217	HOH	OH2	-30.77	-17.16	67.86	15.00
218	HOH	OH2	-30.16	-20.07	64.02	15.00
219	HOH	OH2	-3.64	-10.82	59.75	15.00
220	HOH	OH2	-13.18	-7.77	71.57	15.00
221	HOH	OH2	-34.51	-22.61	70.17	15.00
222	HOH	OH2	-18.02	-34.44	65.29	15.00
223	HOH	OH2	-17.01	-5.28	69.42	15.00
224	HOH	OH2	-24.38	-30.77	62.26	15.00
225	HOH	OH2	0.36	-5.40	64.98	15.00
226	HOH	OH2	-13.68	-21.42	66.86	15.00
227	HOH	OH2	-46.72	-29.80	50.41	15.00
228	HOH	OH2	-45.10	-36.23	56.40	15.00
229	HOH	OH2	-39.09	-12.35	65.48	15.00
230	HOH	OH2	-35.85	-37.05	52.41	15.00
231	HOH	OH2	-19.20	-39.14	66.78	15.00
232	HOH	OH2	-30.09	-19.72	66.64	15.00
233	HOH	OH2	-27.95	-19.50	62.38	15.00
234	HOH	OH2	-21.75	-30.29	62.28	15.00
235	HOH	OH2	-30.30	-2.55	77.57	15.00

TABLE VI

236	HOH	OH2	-33.08	-28.99	86.45	15.00
237	HOH	OH2	-30.07	-22.68	84.37	15.00
238	HOH	OH2	-39.83	-16.82	48.34	15.00
239	HOH	OH2	-34.57	-24.95	47.01	15.00
240	HOH	OH2	-46.44	-34.07	57.12	15.00
241	HOH	OH2	-26.91	-7.02	56.22	15.00
242	HOH	OH2	-42.10	-15.05	61.98	15.00
243	HOH	OH2	-24.27	-7.11	65.05	15.00
244	HOH	OH2	-33.44	-27.69	70.80	15.00
245	HOH	OH2	-40.50	-27.38	80.61	15.00
246	HOH	OH2	-14.45	-17.44	86.64	15.00
247	HOH	OH2	-4.86	-12.23	73.56	15.00
248	HOH	OH2	-10.86	-20.50	79.87	15.00
249	HOH	OH2	-27.43	-35.04	59.25	15.00
250	HOH	OH2	-35.26	-10.90	53.73	15.00
251	HOH	OH2	-31.84	-29.20	46.92	15.00
252	HOH	OH2	-42.75	-9.71	40.49	15.00
253	HOH	OH2	-41.27	-34.56	56.25	15.00
254	HOH	OH2	-44.55	-15.65	65.22	15.00
255	HOH	OH2	-32.52	-13.49	60.73	15.00
256	HOH	OH2	-39.73	-4.62	63.34	15.00
257	HOH	OH2	-25.69	-11.84	70.98	15.00
258	HOH	OH2	-31.93	-6.64	63.98	15.00
259	HOH	OH2	-19.62	-7.72	62.94	15.00
260	HOH	OH2	-33.42	-20.20	70.53	15.00
261	HOH	OH2	-12.62	-24.00	79.04	15.00
262	HOH	OH2	-9.78	-21.46	77.40	15.00
263	HOH	OH2	-6.71	-27.36	80.84	15.00
264	HOH	OH2	-21.06	-35.71	57.19	15.00
265	HOH	OH2	-26.47	-48.97	59.68	15.00
266	HOH	OH2	-14.22	-32.57	69.97	15.00
267	HOH	OH2	-11.69	-25.57	76.63	15.00
268	HOH	OH2	-17.38	-27.79	86.86	15.00
269	HOH	OH2	-22.39	-37.94	70.91	15.00
270	HOH	OH2	-10.44	-11.32	63.69	15.00
271	HOH	OH2	-8.66	-22.33	72.95	15.00
272	HOH	OH2	-29.93	-20.17	48.73	15.00
273	HOH	OH2	-22.92	-30.27	39.30	15.00
274	HOH	OH2	-33.19	-37.20	49.46	15.00
275	HOH	OH2	-28.10	-25.82	41.06	15.00
276	HOH	OH2	-35.93	-29.91	44.54	15.00
277	HOH	OH2	-37.76	-30.41	51.24	15.00

TABLE VII

Table of the orthogonal three dimensional coordinates in
 Angstroms and B factors (\AA^2) for the cathepsin K
 complex with inhibitor 4-[N-
 [(phenylmethoxy)carbonyl]-L-leucyl]-1-[N-
 [(phenylmethoxy)carbonyl]-L-leucyl]-3-
 pyrrolidinone.

Residue Atom	X	Y	Z	B
1 ALA CB	-46.25	-39.17	62.96	30.60
1 ALA C	-47.93	-37.51	63.80	29.74
1 ALA O	-49.14	-37.57	63.58	32.13
1 ALA N	-48.18	-39.83	64.36	28.23
1 ALA CA	-47.15	-38.78	64.13	28.86
2 PRO N	-47.26	-36.34	63.80	27.19
2 PRO CD	-45.94	-36.10	64.40	26.45
2 PRO CA	-47.92	-35.06	63.50	27.01
2 PRO CB	-47.28	-34.10	64.52	26.65
2 PRO CG	-46.25	-34.95	65.31	27.69
2 PRO C	-47.73	-34.52	62.09	26.37
2 PRO O	-46.67	-34.70	61.50	26.53
3 ASP N	-48.76	-33.86	61.58	26.63
3 ASP CA	-48.73	-33.23	60.26	24.49
3 ASP CB	-50.14	-33.03	59.69	23.94
3 ASP CG	-50.75	-34.32	59.17	24.73
3 ASP OD1	-50.19	-34.88	58.21	31.10
3 ASP OD2	-51.79	-34.76	59.71	23.79
3 ASP C	-48.03	-31.88	60.39	24.62
3 ASP O	-47.08	-31.59	59.67	23.92
4 SER N	-48.55	-31.04	61.28	24.05
4 SER CA	-47.98	-29.72	61.55	22.83
4 SER CB	-49.04	-28.62	61.52	23.29
4 SER OG	-49.84	-28.70	60.36	24.54
4 SER C	-47.30	-29.75	62.91	23.31
4 SER O	-47.71	-30.51	63.79	26.63
5 VAL N	-46.27	-28.92	63.09	24.43
5 VAL CA	-45.52	-28.80	64.34	22.41
5 VAL CB	-44.44	-29.91	64.50	24.60
5 VAL CG1	-43.39	-29.50	65.53	19.58
5 VAL CG2	-45.09	-31.22	64.94	26.54
5 VAL C	-44.80	-27.45	64.30	22.72

TABLE VII

5 VAL O	-44.23	-27.09	63.27	24.78
6 ASP N	-44.80	-26.74	65.41	22.25
6 ASP CA	-44.17	-25.43	65.48	20.13
6 ASP CB	-45.15	-24.34	65.04	20.94
6 ASP CG	-44.49	-22.99	64.81	19.46
6 ASP OD1	-43.28	-22.84	65.12	15.02
6 ASP OD2	-45.20	-22.09	64.31	15.42
6 ASP C	-43.67	-25.17	66.88	20.15
6 ASP O	-44.45	-24.78	67.74	26.96
7 TYR N	-42.37	-25.32	67.10	20.70
7 TYR CA	-41.82	-25.08	68.42	19.50
7 TYR CB	-40.44	-25.71	68.58	22.46
7 TYR CG	-40.51	-27.21	68.76	22.69
7 TYR CD1	-40.50	-27.78	70.03	24.39
7 TYR CE1	-40.61	-29.16	70.20	23.01
7 TYR CD2	-40.62	-28.05	67.66	17.84
7 TYR CE2	-40.72	-29.42	67.82	17.55
7 TYR CZ	-40.72	-29.97	69.08	16.70
7 TYR OH	-40.84	-31.33	69.22	21.92
7 TYR C	-41.77	-23.62	68.78	18.59
7 TYR O	-41.12	-23.25	69.75	23.10
8 ARG N	-42.39	-22.78	67.96	16.73
8 ARG CA	-42.44	-21.36	68.25	17.40
8 ARG CB	-42.56	-20.52	66.98	19.28
8 ARG CG	-41.27	-20.40	66.17	22.66
8 ARG CD	-41.41	-19.48	64.98	14.98
8 ARG NE	-42.40	-19.99	64.04	17.92
8 ARG CZ	-42.59	-19.53	62.81	22.05
8 ARG NH1	-41.85	-18.52	62.36	24.53
8 ARG NH2	-43.50	-20.10	62.03	26.01
8 ARG C	-43.64	-21.14	69.17	15.35
8 ARG O	-43.52	-20.55	70.24	14.09
9 LYS N	-44.77	-21.73	68.79	13.90
9 LYS CA	-46.01	-21.63	69.54	13.24
9 LYS CB	-47.21	-21.84	68.62	10.93
9 LYS CG	-47.27	-20.83	67.48	16.03
9 LYS CD	-48.31	-21.19	66.44	13.55
9 LYS CE	-49.69	-21.20	67.04	17.52
9 LYS NZ	-50.71	-21.24	65.97	18.86
9 LYS C	-46.01	-22.61	70.70	15.37
9 LYS O	-47.06	-23.10	71.14	15.03
10 LYS N	-44.81	-22.90	71.19	17.15

TABLE VII

10 LYS CA	-44.58	-23.82	72.31	14.97
10 LYS CB	-44.10	-25.19	71.81	13.68
10 LYS CG	-45.15	-26.06	71.14	17.87
10 LYS CD	-44.58	-27.44	70.87	17.96
10 LYS CE	-45.67	-28.49	70.71	22.08
10 LYS NZ	-45.07	-29.82	70.35	25.39
10 LYS C	-43.52	-23.20	73.23	10.83
10 LYS O	-43.08	-23.82	74.19	9.39
11 GLY N	-43.07	-22.01	72.88	11.15
11 GLY CA	-42.08	-21.35	73.70	14.48
11 GLY C	-40.71	-21.99	73.69	15.75
11 GLY O	-39.92	-21.75	74.60	16.24
12 TYR N	-40.41	-22.80	72.67	16.05
12 TYR CA	-39.09	-23.44	72.59	15.26
12 TYR CB	-39.18	-24.83	71.96	16.85
12 TYR CG	-39.84	-25.90	72.80	12.79
12 TYR CD1	-41.22	-26.04	72.82	12.72
12 TYR CE1	-41.82	-27.07	73.52	16.82
12 TYR CD2	-39.08	-26.82	73.50	18.15
12 TYR CE2	-39.67	-27.86	74.20	21.62
12 TYR CZ	-41.04	-27.98	74.20	19.19
12 TYR OH	-41.63	-29.03	74.89	22.22
12 TYR C	-38.08	-22.61	71.81	16.45
12 TYR O	-36.89	-22.92	71.82	18.97
13 VAL N	-38.55	-21.55	71.16	16.26
13 VAL CA	-37.67	-20.71	70.34	17.11
13 VAL CB	-38.25	-20.58	68.90	17.86
13 VAL CG1	-37.20	-20.07	67.96	18.97
13 VAL CG2	-38.77	-21.92	68.41	19.17
13 VAL C	-37.37	-19.31	70.89	16.02
13 VAL O	-38.27	-18.51	71.14	16.61
14 THR N	-36.08	-19.01	71.03	15.90
14 THR CA	-35.65	-17.71	71.53	20.92
14 THR CB	-34.21	-17.77	72.04	22.63
14 THR OG1	-33.33	-18.11	70.97	28.59
14 THR CG2	-34.09	-18.78	73.17	23.81
14 THR C	-35.73	-16.67	70.41	25.69
14 THR O	-36.01	-17.02	69.26	28.47
15 PRO N	-35.50	-15.37	70.73	28.26
15 PRO CD	-35.15	-14.82	72.05	27.19
15 PRO CA	-35.56	-14.29	69.73	23.60
15 PRO CB	-35.29	-13.04	70.58	24.84

TABLE VII

15 PRO CG	-34.43	-13.55	71.68	26.75
15 PRO C	-34.53	-14.44	68.62	19.41
15 PRO O	-33.43	-14.94	68.84	15.67
16 VAL N	-34.90	-13.96	67.43	16.42
16 VAL CA	-34.03	-14.06	66.27	12.13
16 VAL CB	-34.77	-13.71	64.95	9.20
16 VAL CG1	-33.84	-13.89	63.77	7.84
16 VAL CG2	-36.01	-14.56	64.78	6.59
16 VAL C	-32.81	-13.16	66.39	11.22
16 VAL O	-32.93	-11.94	66.44	11.47
17 LYS N	-31.65	-13.79	66.45	10.35
17 LYS CA	-30.39	-13.07	66.55	9.97
17 LYS CB	-29.31	-13.93	67.22	14.75
17 LYS CG	-29.17	-13.71	68.75	10.18
17 LYS CD	-30.45	-14.02	69.52	5.48
17 LYS CE	-30.69	-15.51	69.66	15.18
17 LYS NZ	-29.75	-16.23	70.59	13.03
17 LYS C	-29.98	-12.57	65.16	9.61
17 LYS O	-30.72	-12.73	64.20	9.93
18 ASN N	-28.76	-12.05	65.05	8.91
18 ASN CA	-28.28	-11.47	63.80	8.23
18 ASN CB	-28.78	-10.03	63.72	10.88
18 ASN CG	-28.51	-9.36	62.39	13.91
18 ASN OD1	-27.51	-9.63	61.72	9.48
18 ASN ND2	-29.40	-8.44	62.03	13.48
18 ASN C	-26.75	-11.54	63.75	8.02
18 ASN O	-26.07	-10.64	64.22	13.56
19 GLN N	-26.22	-12.59	63.14	7.59
19 GLN CA	-24.78	-12.81	63.06	9.07
19 GLN CB	-24.50	-14.08	62.26	11.76
19 GLN CG	-24.91	-14.00	60.81	10.58
19 GLN CD	-24.73	-15.33	60.11	10.05
19 GLN OE1	-25.69	-16.07	59.88	8.08
19 GLN NE2	-23.49	-15.66	59.80	3.31
19 GLN C	-23.84	-11.70	62.60	12.84
19 GLN O	-22.65	-11.71	62.95	14.67
20 GLY N	-24.33	-10.75	61.81	9.97
20 GLY CA	-23.45	-9.68	61.35	9.75
20 GLY C	-22.40	-10.16	60.37	9.12
20 GLY O	-22.56	-11.21	59.74	14.46
21 GLN N	-21.32	-9.40	60.20	10.42
21 GLN CA	-20.28	-9.80	59.25	13.95

TABLE VII

21	GLN	CB	-19.55	-8.58	58.66	13.14
21	GLN	CG	-20.40	-7.79	57.65	12.44
21	GLN	CD	-20.73	-8.61	56.41	13.48
21	GLN	OE1	-19.84	-9.15	55.76	14.90
21	GLN	NE2	-22.02	-8.71	56.08	9.41
21	GLN	C	-19.30	-10.83	59.81	15.26
21	GLN	O	-18.08	-10.64	59.79	16.33
22	CYS	N	-19.86	-11.93	60.29	17.72
22	CYS	CA	-19.10	-13.04	60.86	16.36
22	CYS	C	-19.82	-14.31	60.40	16.07
22	CYS	O	-21.05	-14.39	60.44	8.26
22	CYS	CB	-19.02	-12.91	62.40	16.53
22	CYS	SG	-18.36	-14.33	63.35	15.48
23	GLY	N	-19.04	-15.25	59.83	16.86
23	GLY	CA	-19.59	-16.52	59.35	14.89
23	GLY	C	-19.67	-17.49	60.52	13.50
23	GLY	O	-18.91	-18.45	60.61	11.64
24	SER	N	-20.61	-17.20	61.41	13.66
24	SER	CA	-20.82	-17.99	62.61	14.12
24	SER	CB	-20.65	-17.10	63.84	17.06
24	SER	OG	-21.37	-15.88	63.67	19.58
24	SER	C	-22.18	-18.67	62.64	14.42
24	SER	O	-22.63	-19.12	63.69	15.12
25	CYS	N	-22.83	-18.77	61.48	15.74
25	CYS	CA	-24.16	-19.38	61.40	12.45
25	CYS	CB	-24.61	-19.48	59.92	17.82
25	CYS	SG	-23.46	-20.34	58.77	15.84
25	CYS	C	-24.23	-20.73	62.12	12.21
25	CYS	O	-25.27	-21.09	62.66	8.88
25	INH	C1	-26.76	-10.18	57.23	37.63
25	INH	C2	-25.50	-10.64	57.58	37.16
25	INH	C3	-24.85	-11.61	56.79	34.05
25	INH	C4	-25.45	-12.12	55.64	32.87
25	INH	C5	-26.72	-11.65	55.30	36.05
25	INH	C6	-27.38	-10.68	56.09	37.28
25	INH	C7	-24.76	-13.16	54.79	31.70
25	INH	O8	-24.07	-14.24	55.46	33.18
25	INH	C9	-24.20	-15.65	55.36	32.90
25	INH	O10	-24.83	-16.33	56.19	27.65
25	INH	C11	-23.57	-17.64	54.11	33.43
25	INH	C12	-23.56	-17.98	52.63	29.93
25	INH	C13	-24.79	-17.58	51.82	30.09

TABLE VII

25 INH C14	-24.84	-16.08	51.57	28.76
25 INH C15	-24.70	-18.31	50.53	33.84
25 INH C16	-22.36	-18.24	54.80	34.35
25 INH O17	-21.26	-18.25	54.27	39.78
25 INH N18	-22.58	-18.72	56.02	35.16
25 INH C19	-21.64	-19.29	56.85	29.32
25 INH N20	-23.57	-16.20	54.33	34.33
25 INH C21	-21.16	-20.68	56.54	29.68
25 INH C22	-22.10	-19.32	58.29	26.25
25 INH O23	-22.30	-18.20	58.72	26.33
25 INH C24	-13.39	-26.50	60.06	25.12
25 INH C25	-13.12	-25.19	59.68	26.39
25 INH C26	-14.04	-24.48	58.91	25.10
25 INH C27	-15.23	-25.07	58.52	23.88
25 INH C28	-15.49	-26.37	58.90	24.81
25 INH C29	-14.58	-27.09	59.67	23.22
25 INH C30	-16.20	-24.31	57.66	25.64
25 INH O31	-16.99	-24.94	56.63	26.66
25 INH C32	-18.41	-24.84	56.56	24.33
25 INH O33	-19.08	-25.66	55.96	24.89
25 INH C34	-20.39	-23.56	57.26	25.72
25 INH C35	-21.15	-24.78	57.78	22.12
25 INH C36	-21.80	-25.75	56.80	16.61
25 INH C37	-23.15	-25.25	56.41	15.08
25 INH C38	-21.91	-27.08	57.47	16.77
25 INH C39	-20.56	-22.41	58.25	28.82
25 INH O40	-20.39	-22.62	59.45	37.25
25 INH N41	-20.88	-21.18	57.82	28.59
25 INH C42	-21.00	-20.17	58.81	27.26
25 INH N43	-18.95	-23.81	57.20	25.99
26 TRP N	-23.11	-21.45	62.14	14.10
26 TRP CA	-23.02	-22.74	62.82	15.29
26 TRP CB	-21.66	-23.38	62.56	12.22
26 TRP CG	-20.53	-22.49	62.90	15.74
26 TRP CD2	-19.74	-22.52	64.10	17.65
26 TRP CE2	-18.76	-21.51	63.98	15.49
26 TRP CE3	-19.77	-23.30	65.27	18.53
26 TRP CD1	-20.02	-21.49	62.14	16.57
26 TRP NE1	-18.95	-20.90	62.77	17.92
26 TRP CZ2	-17.82	-21.26	64.98	13.72
26 TRP CZ3	-18.83	-23.05	66.26	16.53
26 TRP CH2	-17.87	-22.04	66.11	15.09

TABLE VII

26	TRP C	-23.24	-22.55	64.32	19.46
26	TRP O	-24.09	-23.21	64.92	24.77
27	ALA N	-22.52	-21.59	64.90	19.49
27	ALA CA	-22.61	-21.25	66.31	12.94
27	ALA CB	-21.77	-20.01	66.61	12.05
27	ALA C	-24.07	-20.99	66.64	8.35
27	ALA O	-24.61	-21.54	67.60	6.75
28	PHE N	-24.72	-20.18	65.80	8.07
28	PHE CA	-26.13	-19.83	65.95	9.51
28	PHE CB	-26.51	-18.67	65.04	7.62
28	PHE CG	-25.96	-17.35	65.48	4.72
28	PHE CD1	-24.74	-16.91	65.01	4.11
28	PHE CD2	-26.66	-16.56	66.38	2.92
28	PHE CE1	-24.22	-15.69	65.41	4.53
28	PHE CE2	-26.16	-15.33	66.79	2.38
28	PHE CZ	-24.93	-14.89	66.31	2.00
28	PHE C	-27.07	-21.01	65.72	10.66
28	PHE O	-28.18	-21.04	66.26	14.07
29	SER N	-26.64	-21.96	64.89	10.83
29	SER CA	-27.44	-23.15	64.62	8.54
29	SER CB	-26.92	-23.88	63.37	2.45
29	SER OG	-27.80	-24.93	62.97	2.00
29	SER C	-27.40	-24.05	65.86	7.86
29	SER O	-28.44	-24.46	66.38	6.37
30	SER N	-26.19	-24.29	66.36	5.14
30	SER CA	-26.00	-25.14	67.52	7.65
30	SER CB	-24.52	-25.27	67.84	10.56
30	SER OG	-23.81	-25.61	66.67	14.28
30	SER C	-26.76	-24.61	68.73	6.72
30	SER O	-27.57	-25.32	69.34	8.64
31	VAL N	-26.50	-23.35	69.06	6.44
31	VAL CA	-27.15	-22.71	70.19	6.61
31	VAL CB	-26.73	-21.23	70.25	6.76
31	VAL CG1	-27.74	-20.40	71.03	9.71
31	VAL CG2	-25.35	-21.14	70.90	2.00
31	VAL C	-28.67	-22.86	70.18	9.86
31	VAL O	-29.25	-23.30	71.17	13.64
32	GLY N	-29.30	-22.56	69.05	12.98
32	GLY CA	-30.75	-22.68	68.94	9.41
32	GLY C	-31.27	-24.10	69.19	10.59
32	GLY O	-32.42	-24.29	69.59	8.20
33	ALA N	-30.44	-25.10	68.91	11.42

TABLE VII

33 ALA CA	-30.82	-26.50	69.12	13.15
33 ALA CB	-29.82	-27.42	68.47	10.51
33 ALA C	-30.86	-26.73	70.64	14.58
33 ALA O	-31.87	-27.19	71.19	12.75
34 LEU N	-29.75	-26.39	71.29	12.77
34 LEU CA	-29.62	-26.51	72.73	12.38
34 LEU CB	-28.26	-26.01	73.20	4.32
34 LEU CG	-27.04	-26.64	72.57	4.80
34 LEU CD1	-25.82	-25.86	72.95	6.27
34 LEU CD2	-26.92	-28.09	73.01	4.63
34 LEU C	-30.73	-25.73	73.43	16.38
34 LEU O	-31.32	-26.22	74.39	18.32
35 GLU N	-31.00	-24.53	72.95	15.34
35 GLU CA	-32.03	-23.71	73.54	15.20
35 GLU CB	-32.17	-22.38	72.81	12.21
35 GLU CG	-30.92	-21.55	72.88	18.17
35 GLU CD	-31.07	-20.22	72.17	21.50
35 GLU OE1	-31.87	-20.14	71.21	23.90
35 GLU OE2	-30.40	-19.25	72.57	22.09
35 GLU C	-33.37	-24.43	73.60	18.81
35 GLU O	-34.06	-24.37	74.62	23.06
36 GLY N	-33.73	-25.11	72.52	19.33
36 GLY CA	-35.00	-25.83	72.48	19.77
36 GLY C	-34.96	-27.02	73.42	21.74
36 GLY O	-35.97	-27.38	74.05	18.02
37 GLN N	-33.79	-27.63	73.53	23.70
37 GLN CA	-33.61	-28.77	74.41	23.25
37 GLN CB	-32.27	-29.48	74.15	22.37
37 GLN CG	-32.08	-29.98	72.71	26.26
37 GLN CD	-33.38	-30.28	71.94	30.06
37 GLN OE1	-34.20	-31.11	72.36	29.64
37 GLN NE2	-33.58	-29.57	70.83	31.26
37 GLN C	-33.73	-28.32	75.86	24.67
37 GLN O	-34.51	-28.89	76.62	25.08
38 LEU N	-32.99	-27.27	76.22	22.29
38 LEU CA	-33.04	-26.73	77.57	23.08
38 LEU CB	-32.20	-25.46	77.70	21.38
38 LEU CG	-32.11	-24.78	79.07	17.48
38 LEU CD1	-31.77	-25.77	80.17	13.71
38 LEU CD2	-31.07	-23.68	78.99	17.90
38 LEU C	-34.47	-26.46	77.99	24.35
38 LEU O	-34.92	-26.97	79.01	26.24

TABLE VII

39 LYS N	-35.20	-25.71	77.17	26.25
39 LYS CA	-36.59	-25.41	77.47	28.16
39 LYS CB	-37.25	-24.61	76.34	28.65
39 LYS CG	-38.35	-23.65	76.81	27.61
39 LYS CD	-39.60	-24.37	77.25	27.20
39 LYS CE	-40.68	-23.40	77.70	26.81
39 LYS NZ	-41.94	-24.12	78.05	28.10
39 LYS C	-37.37	-26.69	77.76	26.01
39 LYS O	-38.28	-26.70	78.60	25.82
40 LYS N	-37.00	-27.77	77.11	26.61
40 LYS CA	-37.69	-29.03	77.34	27.03
40 LYS CB	-37.64	-29.93	76.11	28.30
40 LYS CG	-38.65	-31.06	76.16	29.91
40 LYS CD	-38.79	-31.77	74.82	29.72
40 LYS CE	-37.74	-32.83	74.61	26.31
40 LYS NZ	-38.04	-33.61	73.37	31.45
40 LYS C	-37.09	-29.72	78.56	25.36
40 LYS O	-37.81	-30.32	79.35	23.91
41 LYS N	-35.78	-29.57	78.73	25.39
41 LYS CA	-35.06	-30.20	79.84	25.65
41 LYS CB	-33.55	-30.06	79.66	24.57
41 LYS CG	-32.72	-30.84	80.67	20.75
41 LYS CD	-32.89	-32.34	80.50	26.88
41 LYS CE	-31.76	-33.13	81.15	28.72
41 LYS NZ	-31.63	-32.85	82.61	29.46
41 LYS C	-35.50	-29.67	81.19	25.70
41 LYS O	-35.92	-30.44	82.06	23.51
42 THR N	-35.42	-28.35	81.34	26.91
42 THR CA	-35.76	-27.67	82.58	25.94
42 THR CB	-34.61	-26.77	83.03	26.05
42 THR OG1	-34.60	-25.58	82.23	27.18
42 THR CG2	-33.28	-27.49	82.85	28.99
42 THR C	-37.00	-26.78	82.52	25.00
42 THR O	-37.57	-26.43	83.55	28.90
43 GLY N	-37.38	-26.35	81.32	24.41
43 GLY CA	-38.54	-25.48	81.19	21.01
43 GLY C	-38.09	-24.02	81.13	19.83
43 GLY O	-38.92	-23.10	81.08	14.91
44 LYS N	-36.78	-23.82	81.15	22.11
44 LYS CA	-36.16	-22.50	81.10	24.14
44 LYS CB	-35.06	-22.38	82.17	26.33
44 LYS CG	-35.61	-22.19	83.60	25.46

TABLE VII

44 LYS CD	-34.54	-22.37	84.69	26.23
44 LYS CE	-33.36	-21.39	84.56	26.78
44 LYS NZ	-32.26	-21.89	83.66	25.35
44 LYS C	-35.63	-22.16	79.70	22.98
44 LYS O	-34.86	-22.92	79.12	25.51
45 LEU N	-36.06	-21.02	79.17	20.83
45 LEU CA	-35.68	-20.55	77.84	14.37
45 LEU CB	-36.93	-20.19	77.03	6.57
45 LEU CG	-36.73	-19.98	75.54	7.56
45 LEU CD1	-36.34	-21.28	74.88	7.35
45 LEU CD2	-38.01	-19.44	74.92	7.68
45 LEU C	-34.73	-19.36	77.92	12.93
45 LEU O	-35.17	-18.22	78.02	12.18
46 LEU N	-33.43	-19.62	77.91	12.78
46 LEU CA	-32.45	-18.55	77.99	16.27
46 LEU CB	-31.57	-18.68	79.23	17.06
46 LEU CG	-32.20	-18.84	80.61	22.73
46 LEU CD1	-33.29	-17.80	80.80	27.00
46 LEU CD2	-32.76	-20.25	80.75	24.49
46 LEU C	-31.59	-18.55	76.75	19.40
46 LEU O	-31.38	-19.61	76.15	22.78
47 ASN N	-31.05	-17.39	76.39	19.21
47 ASN CA	-30.18	-17.27	75.21	16.88
47 ASN CB	-30.12	-15.82	74.70	17.63
47 ASN CG	-31.41	-15.38	74.02	19.44
47 ASN OD1	-32.47	-15.31	74.64	24.63
47 ASN ND2	-31.33	-15.04	72.74	18.95
47 ASN C	-28.78	-17.79	75.50	14.05
47 ASN O	-28.08	-17.23	76.36	11.81
48 LEU N	-28.39	-18.87	74.83	12.40
48 LEU CA	-27.05	-19.46	74.97	13.22
48 LEU CB	-27.02	-20.94	74.58	14.23
48 LEU CG	-27.64	-22.02	75.50	16.25
48 LEU CD1	-26.96	-22.02	76.87	20.21
48 LEU CD2	-29.13	-21.80	75.67	14.71
48 LEU C	-26.08	-18.63	74.14	13.45
48 LEU O	-26.51	-17.85	73.29	17.95
49 SER N	-24.78	-18.80	74.36	15.33
49 SER CA	-23.79	-17.98	73.65	13.70
49 SER CB	-22.77	-17.41	74.65	14.72
49 SER OG	-21.73	-16.68	74.02	13.12
49 SER C	-23.05	-18.50	72.42	14.35

TABLE VII

49	SER O	-22.14	-19.33	72.52	15.35
50	PRO N	-23.38	-17.93	71.24	13.10
50	PRO CD	-24.49	-16.99	71.00	13.10
50	PRO CA	-22.73	-18.30	69.99	8.82
50	PRO CB	-23.41	-17.39	68.98	10.23
50	PRO CG	-24.79	-17.23	69.54	10.20
50	PRO C	-21.25	-17.95	70.09	7.83
50	PRO O	-20.40	-18.65	69.56	7.76
51	GLN N	-20.96	-16.86	70.80	8.14
51	GLN CA	-19.59	-16.38	70.97	8.89
51	GLN CB	-19.58	-14.99	71.62	12.14
51	GLN CG	-18.31	-14.16	71.33	13.72
51	GLN CD	-18.18	-13.71	69.87	12.95
51	GLN OE1	-19.12	-13.18	69.27	10.44
51	GLN NE2	-16.99	-13.89	69.30	6.01
51	GLN C	-18.70	-17.34	71.74	8.59
51	GLN O	-17.49	-17.46	71.45	8.17
52	ASN N	-19.27	-18.03	72.72	6.61
52	ASN CA	-18.50	-19.01	73.49	6.19
52	ASN CB	-19.36	-19.58	74.62	6.41
52	ASN CG	-18.70	-20.74	75.34	7.63
52	ASN OD1	-19.39	-21.64	75.81	9.07
52	ASN ND2	-17.39	-20.70	75.48	4.94
52	ASN C	-18.04	-20.09	72.50	9.66
52	ASN O	-16.89	-20.56	72.54	9.03
53	LEU N	-18.94	-20.43	71.58	10.50
53	LEU CA	-18.69	-21.42	70.54	7.20
53	LEU CB	-20.01	-21.83	69.89	6.76
53	LEU CG	-20.74	-23.04	70.49	12.00
53	LEU CD1	-20.47	-23.19	71.98	14.61
53	LEU CD2	-22.22	-22.93	70.21	8.55
53	LEU C	-17.69	-20.92	69.49	6.03
53	LEU O	-16.75	-21.63	69.14	4.01
54	VAL N	-17.87	-19.70	69.01	2.00
54	VAL CA	-16.99	-19.14	68.00	6.81
54	VAL CB	-17.34	-17.67	67.64	7.05
54	VAL CG1	-16.27	-17.07	66.74	13.23
54	VAL CG2	-18.66	-17.58	66.93	5.36
54	VAL C	-15.55	-19.15	68.47	12.15
54	VAL O	-14.66	-19.63	67.76	16.44
55	ASP N	-15.32	-18.59	69.65	15.93
55	ASP CA	-13.98	-18.48	70.22	17.26

TABLE VII

55 ASP CB	-13.98	-17.47	71.37	19.77
55 ASP CG	-14.33	-16.06	70.94	22.96
55 ASP OD1	-14.48	-15.78	69.72	24.84
55 ASP OD2	-14.44	-15.21	71.84	23.39
55 ASP C	-13.37	-19.78	70.72	18.42
55 ASP O	-12.18	-20.06	70.49	12.75
56 CYS N	-14.18	-20.55	71.43	20.14
56 CYS CA	-13.75	-21.79	72.06	19.35
56 CYS C	-13.66	-23.12	71.30	16.79
56 CYS O	-13.00	-24.05	71.77	19.07
56 CYS CB	-14.52	-21.96	73.37	17.64
56 CYS SG	-14.48	-20.45	74.39	15.52
57 VAL N	-14.31	-23.23	70.14	14.99
57 VAL CA	-14.24	-24.47	69.38	12.09
57 VAL CB	-15.48	-24.72	68.51	9.25
57 VAL CG1	-15.37	-26.09	67.85	2.60
57 VAL CG2	-16.75	-24.62	69.34	5.09
57 VAL C	-13.02	-24.48	68.47	12.69
57 VAL O	-13.04	-23.91	67.39	15.30
58 SER N	-11.96	-25.14	68.92	15.12
58 SER CA	-10.72	-25.21	68.15	18.94
58 SER CB	-9.59	-25.78	69.00	21.08
58 SER OG	-9.92	-27.07	69.49	20.89
58 SER C	-10.84	-25.98	66.83	19.38
58 SER O	-10.00	-25.81	65.94	21.21
59 GLU N	-11.83	-26.87	66.74	21.74
59 GLU CA	-12.04	-27.68	65.53	20.63
59 GLU CB	-12.88	-28.94	65.82	20.59
59 GLU CG	-12.48	-29.76	67.06	21.89
59 GLU CD	-13.08	-29.21	68.37	21.83
59 GLU OE1	-14.32	-29.11	68.47	25.51
59 GLU OE2	-12.31	-28.90	69.30	26.68
59 GLU C	-12.69	-26.87	64.41	19.86
59 GLU O	-12.56	-27.21	63.23	21.27
60 ASN N	-13.43	-25.83	64.79	16.86
60 ASN CA	-14.11	-24.97	63.83	10.64
60 ASN CB	-15.49	-24.61	64.33	2.00
60 ASN CG	-16.43	-25.78	64.27	6.50
60 ASN OD1	-17.46	-25.83	64.96	3.71
60 ASN ND2	-16.09	-26.75	63.42	3.21
60 ASN C	-13.27	-23.76	63.49	13.09
60 ASN O	-12.25	-23.51	64.13	14.35

TABLE VII

61 ASP N	-13.67	-23.01	62.46	14.85
61 ASP CA	-12.90	-21.86	62.02	15.28
61 ASP CB	-12.74	-21.86	60.51	21.27
61 ASP CG	-11.30	-22.08	60.07	23.24
61 ASP OD1	-10.60	-21.08	59.84	26.41
61 ASP OD2	-10.88	-23.25	59.97	20.64
61 ASP C	-13.36	-20.50	62.51	15.18
61 ASP O	-12.89	-19.47	62.01	13.47
62 GLY N	-14.26	-20.50	63.48	15.64
62 GLY CA	-14.75	-19.25	64.03	15.74
62 GLY C	-15.68	-18.55	63.07	17.26
62 GLY O	-16.72	-19.10	62.72	19.72
63 CYS N	-15.30	-17.35	62.64	19.00
63 CYS CA	-16.14	-16.62	61.70	18.17
63 CYS C	-16.00	-17.19	60.29	19.74
63 CYS O	-16.79	-16.86	59.41	22.59
63 CYS CB	-15.85	-15.11	61.73	16.37
63 CYS SG	-16.32	-14.21	63.25	14.06
64 GLY N	-15.00	-18.05	60.09	17.99
64 GLY CA	-14.81	-18.67	58.79	15.84
64 GLY C	-15.66	-19.92	58.60	17.59
64 GLY O	-15.50	-20.66	57.63	19.05
65 GLY N	-16.59	-20.15	59.53	18.26
65 GLY CA	-17.46	-21.31	59.44	12.24
65 GLY C	-17.03	-22.45	60.34	10.78
65 GLY O	-15.90	-22.47	60.83	9.37
66 GLY N	-17.94	-23.40	60.53	8.77
66 GLY CA	-17.68	-24.56	61.36	8.46
66 GLY C	-18.83	-25.55	61.24	10.14
66 GLY O	-19.79	-25.29	60.51	9.60
67 TYR N	-18.69	-26.70	61.88	12.33
67 TYR CA	-19.74	-27.73	61.84	14.13
67 TYR CB	-19.18	-29.12	61.49	14.00
67 TYR CG	-18.53	-29.22	60.13	16.82
67 TYR CD1	-19.29	-29.29	58.96	19.29
67 TYR CE1	-18.68	-29.37	57.70	19.34
67 TYR CD2	-17.15	-29.24	60.02	17.85
67 TYR CE2	-16.53	-29.32	58.77	21.15
67 TYR CZ	-17.30	-29.39	57.61	22.41
67 TYR OH	-16.66	-29.42	56.38	22.94
67 TYR C	-20.44	-27.77	63.20	12.95
67 TYR O	-19.80	-27.61	64.23	14.93

TABLE VII

68 MET N	-21.75	-27.98	63.19	14.10
68 MET CA	-22.51	-28.01	64.44	11.02
68 MET CB	-24.02	-28.04	64.18	7.28
68 MET CG	-24.57	-26.75	63.53	12.57
68 MET SD	-24.82	-26.81	61.72	9.43
68 MET CE	-23.29	-26.23	61.15	5.50
68 MET C	-22.07	-29.15	65.34	10.25
68 MET O	-21.98	-28.98	66.55	9.78
69 THR N	-21.74	-30.30	64.76	11.11
69 THR CA	-21.31	-31.45	65.54	9.38
69 THR CB	-21.06	-32.69	64.65	7.39
69 THR OG1	-20.19	-32.36	63.55	6.10
69 THR CG2	-22.39	-33.24	64.11	6.49
69 THR C	-20.08	-31.11	66.39	8.98
69 THR O	-20.06	-31.41	67.57	15.86
70 ASN N	-19.09	-30.44	65.81	5.69
70 ASN CA	-17.89	-30.06	66.55	7.38
70 ASN CB	-16.87	-29.34	65.67	9.34
70 ASN CG	-16.43	-30.17	64.49	11.35
70 ASN OD1	-16.13	-29.63	63.43	13.75
70 ASN ND2	-16.38	-31.48	64.66	13.26
70 ASN C	-18.26	-29.15	67.71	9.60
70 ASN O	-17.68	-29.25	68.79	10.75
71 ALA N	-19.24	-28.28	67.47	12.80
71 ALA CA	-19.72	-27.33	68.48	15.69
71 ALA CB	-20.62	-26.29	67.84	12.87
71 ALA C	-20.48	-28.04	69.59	16.01
71 ALA O	-20.50	-27.56	70.72	18.32
72 PHE N	-21.14	-29.14	69.25	15.89
72 PHE CA	-21.91	-29.90	70.23	15.72
72 PHE CB	-22.88	-30.85	69.53	12.85
72 PHE CG	-24.07	-30.17	68.91	10.89
72 PHE CD1	-24.61	-29.03	69.48	13.23
72 PHE CD2	-24.69	-30.70	67.78	13.69
72 PHE CE1	-25.75	-28.43	68.93	14.17
72 PHE CE2	-25.83	-30.10	67.23	11.57
72 PHE CZ	-26.36	-28.96	67.80	8.27
72 PHE C	-20.93	-30.66	71.11	17.93
72 PHE O	-20.98	-30.59	72.34	16.27
73 GLN N	-20.01	-31.36	70.44	19.40
73 GLN CA	-18.97	-32.16	71.08	19.37
73 GLN CB	-18.09	-32.78	70.00	17.22

TABLE VII

73 GLN CG	-16.99	-33.70	70.46	19.79
73 GLN CD	-16.30	-34.36	69.27	20.51
73 GLN OE1	-16.73	-35.40	68.78	22.61
73 GLN NE2	-15.24	-33.72	68.75	18.71
73 GLN C	-18.15	-31.29	72.03	20.01
73 GLN O	-17.74	-31.75	73.10	20.37
74 TYR N	-17.92	-30.04	71.65	18.39
74 TYR CA	-17.16	-29.12	72.48	15.45
74 TYR CB	-16.90	-27.79	71.73	13.54
74 TYR CG	-16.82	-26.58	72.63	12.20
74 TYR CD1	-15.63	-26.22	73.26	10.63
74 TYR CE1	-15.59	-25.18	74.18	11.99
74 TYR CD2	-17.97	-25.84	72.93	9.97
74 TYR CE2	-17.94	-24.79	73.84	7.22
74 TYR CZ	-16.75	-24.47	74.47	11.24
74 TYR OH	-16.74	-23.48	75.43	17.85
74 TYR C	-17.93	-28.93	73.80	12.38
74 TYR O	-17.38	-29.14	74.87	15.74
75 VAL N	-19.21	-28.60	73.71	11.39
75 VAL CA	-20.05	-28.38	74.88	11.24
75 VAL CB	-21.50	-28.06	74.44	8.02
75 VAL CG1	-22.42	-27.95	75.64	6.92
75 VAL CG2	-21.54	-26.76	73.66	9.76
75 VAL C	-20.05	-29.59	75.83	16.34
75 VAL O	-20.35	-29.45	77.03	11.43
76 GLN N	-19.74	-30.76	75.28	18.49
76 GLN CA	-19.69	-32.02	76.03	17.15
76 GLN CB	-19.98	-33.22	75.11	16.55
76 GLN CG	-19.90	-34.60	75.78	17.80
76 GLN CD	-20.05	-35.78	74.81	16.42
76 GLN OE1	-19.33	-35.89	73.81	12.60
76 GLN NE2	-20.98	-36.68	75.12	11.09
76 GLN C	-18.33	-32.15	76.71	17.72
76 GLN O	-18.25	-32.28	77.92	19.51
77 LYS N	-17.25	-32.04	75.94	18.51
77 LYS CA	-15.91	-32.16	76.50	18.56
77 LYS CB	-14.84	-32.18	75.41	18.21
77 LYS CG	-14.75	-33.47	74.62	18.16
77 LYS CD	-13.48	-33.47	73.77	21.11
77 LYS CE	-13.38	-34.69	72.84	22.51
77 LYS NZ	-12.02	-34.81	72.23	21.73
77 LYS C	-15.58	-31.08	77.52	20.04

TABLE VII

77 LYS O	-14.76	-31.29	78.42	21.61
78 ASN N	-16.20	-29.91	77.36	20.45
78 ASN CA	-15.96	-28.79	78.27	19.68
78 ASN CB	-15.88	-27.47	77.50	18.78
78 ASN CG	-15.19	-26.36	78.30	19.30
78 ASN OD1	-13.97	-26.34	78.44	16.41
78 ASN ND2	-15.98	-25.40	78.79	20.55
78 ASN C	-17.03	-28.73	79.35	18.44
78 ASN O	-17.03	-27.83	80.18	20.10
79 ARG N	-17.96	-29.68	79.32	16.26
79 ARG CA	-19.04	-29.74	80.30	16.53
79 ARG CB	-18.53	-30.31	81.63	16.34
79 ARG CG	-17.65	-31.54	81.47	17.65
79 ARG CD	-16.99	-31.93	82.78	19.26
79 ARG NE	-16.03	-33.01	82.58	21.25
79 ARG CZ	-14.74	-32.82	82.27	24.36
79 ARG NH1	-14.27	-31.59	82.11	27.69
79 ARG NH2	-13.93	-33.86	82.13	18.73
79 ARG C	-19.74	-28.39	80.51	14.94
79 ARG O	-19.91	-27.95	81.64	14.77
80 GLY N	-20.12	-27.73	79.42	16.45
80 GLY CA	-20.82	-26.46	79.56	14.39
80 GLY C	-20.59	-25.34	78.56	13.10
80 GLY O	-19.49	-25.18	78.00	10.43
81 ILE N	-21.64	-24.54	78.38	9.15
81 ILE CA	-21.62	-23.39	77.50	7.25
81 ILE CB	-22.39	-23.68	76.19	6.85
81 ILE CG2	-23.87	-23.89	76.48	4.07
81 ILE CG1	-22.16	-22.55	75.18	8.21
81 ILE CD1	-23.07	-22.63	73.97	11.83
81 ILE C	-22.27	-22.21	78.25	8.64
81 ILE O	-23.29	-22.38	78.94	9.51
82 ASP N	-21.68	-21.03	78.13	11.32
82 ASP CA	-22.20	-19.84	78.81	12.61
82 ASP CB	-21.14	-18.75	78.92	10.86
82 ASP CG	-19.95	-19.18	79.72	10.55
82 ASP OD1	-18.81	-18.86	79.31	8.90
82 ASP OD2	-20.14	-19.86	80.74	14.89
82 ASP C	-23.46	-19.26	78.19	12.50
82 ASP O	-23.92	-19.70	77.14	15.36
83 SER N	-24.03	-18.28	78.87	11.91
83 SER CA	-25.23	-17.61	78.39	12.55

TABLE VII

83	SER CB	-26.14	-17.24	79.55	18.80
83	SER OG	-25.48	-16.36	80.45	22.70
83	SER C	-24.78	-16.35	77.64	9.20
83	SER O	-23.59	-16.01	77.64	5.74
84	GLU N	-25.71	-15.67	76.99	9.19
84	GLU CA	-25.33	-14.43	76.31	14.72
84	GLU CB	-26.47	-13.88	75.45	13.64
84	GLU CG	-26.29	-14.13	73.96	13.53
84	GLU CD	-25.09	-13.41	73.36	12.40
84	GLU OE1	-24.88	-12.23	73.68	14.45
84	GLU OE2	-24.38	-14.02	72.56	16.00
84	GLU C	-24.86	-13.42	77.35	15.76
84	GLU O	-23.85	-12.75	77.16	15.77
85	ASP N	-25.57	-13.36	78.49	18.15
85	ASP CA	-25.21	-12.45	79.58	18.14
85	ASP CB	-26.05	-12.73	80.84	21.42
85	ASP CG	-27.47	-12.20	80.72	27.07
85	ASP OD1	-28.43	-12.97	80.98	25.69
85	ASP OD2	-27.63	-11.01	80.38	28.79
85	ASP C	-23.73	-12.56	79.90	20.03
85	ASP O	-22.98	-11.59	79.78	24.76
86	ALA N	-23.32	-13.77	80.28	17.91
86	ALA CA	-21.93	-14.08	80.62	16.67
86	ALA CB	-21.87	-15.44	81.30	15.93
86	ALA C	-20.99	-14.07	79.41	19.50
86	ALA O	-19.76	-14.03	79.57	22.48
87	TYR N	-21.56	-14.13	78.21	16.64
87	TYR CA	-20.72	-14.15	77.01	16.44
87	TYR CB	-20.31	-15.59	76.69	12.21
87	TYR CG	-18.90	-15.72	76.20	5.93
87	TYR CD1	-18.37	-14.81	75.28	6.36
87	TYR CE1	-17.08	-14.96	74.80	2.57
87	TYR CD2	-18.10	-16.78	76.62	7.25
87	TYR CE2	-16.81	-16.93	76.14	3.11
87	TYR CZ	-16.31	-16.01	75.23	2.00
87	TYR OH	-15.04	-16.18	74.72	8.83
87	TYR C	-21.41	-13.49	75.82	16.77
87	TYR O	-21.87	-14.18	74.91	22.23
88	PRO N	-21.48	-12.15	75.80	15.42
88	PRO CD	-20.91	-11.18	76.74	12.94
88	PRO CA	-22.13	-11.44	74.70	13.08
88	PRO CB	-21.96	-9.97	75.08	12.38

TABLE VII

88 PRO CG	-21.82	-10.00	76.55	9.35
88 PRO C	-21.49	-11.72	73.35	14.00
88 PRO O	-20.33	-12.14	73.27	15.05
89 TYR N	-22.25	-11.52	72.28	13.57
89 TYR CA	-21.77	-11.73	70.93	14.96
89 TYR CB	-22.90	-12.16	69.99	16.79
89 TYR CG	-22.46	-12.46	68.56	19.46
89 TYR CD1	-21.64	-13.54	68.28	17.96
89 TYR CE1	-21.26	-13.85	66.98	20.62
89 TYR CD2	-22.90	-11.67	67.49	17.49
89 TYR CE2	-22.53	-11.96	66.17	17.03
89 TYR CZ	-21.70	-13.06	65.92	17.44
89 TYR OH	-21.28	-13.36	64.65	16.20
89 TYR C	-21.11	-10.47	70.39	14.19
89 TYR O	-21.79	-9.45	70.23	14.43
90 VAL N	-19.80	-10.50	70.18	11.92
90 VAL CA	-19.15	-9.33	69.61	12.81
90 VAL CB	-17.69	-9.13	70.09	11.22
90 VAL CG1	-17.68	-8.76	71.57	19.09
90 VAL CG2	-16.84	-10.35	69.83	10.92
90 VAL C	-19.21	-9.39	68.09	14.23
90 VAL O	-19.09	-8.36	67.42	14.19
91 GLY N	-19.44	-10.58	67.53	14.09
91 GLY CA	-19.52	-10.72	66.09	15.26
91 GLY C	-18.16	-10.68	65.44	18.32
91 GLY O	-18.01	-10.38	64.24	16.36
92 GLN N	-17.16	-11.06	66.23	20.31
92 GLN CA	-15.78	-11.06	65.81	20.17
92 GLN CB	-15.16	-9.69	66.09	23.65
92 GLN CG	-13.83	-9.44	65.42	28.99
92 GLN CD	-13.36	-8.00	65.62	34.47
92 GLN OE1	-14.10	-7.15	66.15	34.75
92 GLN NE2	-12.14	-7.72	65.19	37.63
92 GLN C	-15.09	-12.17	66.60	20.89
92 GLN O	-15.53	-12.53	67.70	18.43
93 GLU N	-14.04	-12.73	66.03	22.82
93 GLU CA	-13.31	-13.81	66.69	24.92
93 GLU CB	-12.63	-14.74	65.66	27.98
93 GLU CG	-12.23	-16.10	66.22	29.38
93 GLU CD	-12.00	-17.17	65.15	34.25
93 GLU OE1	-12.30	-16.93	63.95	35.80
93 GLU OE2	-11.52	-18.26	65.52	34.14

TABLE VII

93 GLU C	-12.31	-13.29	67.71	24.19
93 GLU O	-11.61	-12.31	67.45	24.56
94 GLU N	-12.28	-13.94	68.87	23.61
94 GLU CA	-11.38	-13.58	69.96	24.32
94 GLU CB	-12.02	-12.55	70.90	22.62
94 GLU CG	-12.23	-11.20	70.27	23.90
94 GLU CD	-12.86	-10.23	71.21	24.44
94 GLU OE1	-12.18	-9.26	71.60	29.56
94 GLU OE2	-14.04	-10.43	71.57	23.54
94 GLU C	-10.99	-14.84	70.73	23.80
94 GLU O	-11.64	-15.89	70.59	21.98
95 SER N	-9.95	-14.73	71.55	20.75
95 SER CA	-9.47	-15.86	72.36	19.71
95 SER CB	-8.26	-15.46	73.19	20.00
95 SER OG	-8.57	-14.41	74.09	24.28
95 SER C	-10.60	-16.38	73.25	20.63
95 SER O	-11.48	-15.60	73.65	22.33
96 CYS N	-10.56	-17.66	73.58	17.74
96 CYS CA	-11.60	-18.26	74.42	18.66
96 CYS C	-11.59	-17.72	75.85	19.92
96 CYS O	-10.58	-17.79	76.56	21.50
96 CYS CB	-11.51	-19.78	74.41	16.39
96 CYS SG	-12.75	-20.61	75.44	19.58
97 MET N	-12.72	-17.14	76.26	17.89
97 MET CA	-12.88	-16.59	77.60	18.67
97 MET CB	-12.86	-15.07	77.57	17.60
97 MET CG	-12.76	-14.43	78.94	18.29
97 MET SD	-11.15	-13.66	79.17	26.40
97 MET CE	-9.99	-15.01	78.76	19.16
97 MET C	-14.18	-17.09	78.20	21.66
97 MET O	-15.07	-16.31	78.52	25.61
98 TYR N	-14.30	-18.41	78.29	23.47
98 TYR CA	-15.49	-19.06	78.83	23.75
98 TYR CB	-15.58	-20.50	78.30	21.70
98 TYR CG	-16.39	-21.46	79.13	18.51
98 TYR CD1	-17.74	-21.64	78.90	18.20
98 TYR CE1	-18.49	-22.49	79.70	19.99
98 TYR CD2	-15.80	-22.16	80.17	16.39
98 TYR CE2	-16.53	-23.01	80.97	12.68
98 TYR CZ	-17.87	-23.17	80.74	16.90
98 TYR OH	-18.60	-23.99	81.57	22.57
98 TYR C	-15.48	-19.01	80.37	26.07

TABLE VII

98 TYR O	-14.44	-19.23	80.99	27.32
99 ASN N	-16.63	-18.67	80.96	28.21
99 ASN CA	-16.76	-18.59	82.42	27.40
99 ASN CB	-17.24	-17.20	82.85	30.57
99 ASN CG	-17.89	-17.21	84.22	33.86
99 ASN OD1	-19.06	-16.84	84.36	33.41
99 ASN ND2	-17.16	-17.66	85.24	34.39
99 ASN C	-17.67	-19.66	83.03	25.48
99 ASN O	-18.88	-19.64	82.82	25.31
100 PRO N	-17.12	-20.53	83.87	22.21
100 PRO CD	-15.70	-20.60	84.27	21.06
100 PRO CA	-17.89	-21.60	84.50	19.72
100 PRO CB	-16.89	-22.18	85.49	21.18
100 PRO CG	-15.58	-22.01	84.75	22.13
100 PRO C	-19.14	-21.08	85.22	19.80
100 PRO O	-20.22	-21.65	85.09	15.82
101 THR N	-18.98	-19.97	85.92	22.73
101 THR CA	-20.07	-19.36	86.68	23.85
101 THR CB	-19.53	-18.25	87.60	22.86
101 THR OG1	-18.13	-18.47	87.87	20.58
101 THR CG2	-20.28	-18.26	88.92	21.48
101 THR C	-21.22	-18.80	85.82	24.75
101 THR O	-22.30	-18.46	86.33	22.15
102 GLY N	-20.96	-18.70	84.51	25.15
102 GLY CA	-21.96	-18.20	83.59	21.81
102 GLY C	-22.72	-19.34	82.94	19.11
102 GLY O	-23.78	-19.12	82.36	19.57
103 LYS N	-22.15	-20.55	83.03	18.20
103 LYS CA	-22.73	-21.77	82.47	16.81
103 LYS CB	-22.08	-23.02	83.07	16.94
103 LYS CG	-22.90	-24.30	82.93	15.32
103 LYS CD	-22.03	-25.53	83.10	18.87
103 LYS CE	-21.32	-25.57	84.46	21.19
103 LYS NZ	-20.02	-26.34	84.40	20.74
103 LYS C	-24.24	-21.83	82.62	17.92
103 LYS O	-24.78	-21.68	83.72	18.81
104 ALA N	-24.92	-22.05	81.50	17.95
104 ALA CA	-26.38	-22.11	81.49	17.78
104 ALA CB	-26.93	-21.14	80.47	21.54
104 ALA C	-26.84	-23.52	81.18	18.07
104 ALA O	-27.99	-23.88	81.47	16.81
105 ALA N	-25.95	-24.31	80.58	15.87

TABLE VII

105 ALA CA	-26.27	-25.69	80.23	13.04
105 ALA CB	-27.41	-25.72	79.22	10.01
105 ALA C	-25.05	-26.40	79.66	11.95
105 ALA O	-23.94	-25.86	79.68	8.46
106 LYS N	-25.27	-27.63	79.20	12.25
106 LYS CA	-24.24	-28.45	78.57	18.76
106 LYS CB	-23.26	-29.07	79.58	23.73
106 LYS CG	-23.89	-30.02	80.60	26.39
106 LYS CD	-22.88	-31.05	81.09	29.44
106 LYS CE	-23.54	-32.05	82.06	33.28
106 LYS NZ	-24.76	-32.74	81.51	24.10
106 LYS C	-24.95	-29.54	77.77	18.52
106 LYS O	-26.18	-29.49	77.64	16.87
107 CYS N	-24.21	-30.50	77.22	19.97
107 CYS CA	-24.81	-31.59	76.45	21.83
107 CYS CB	-25.13	-31.16	75.00	23.15
107 CYS SG	-23.72	-30.88	73.87	21.75
107 CYS C	-23.98	-32.87	76.48	22.08
107 CYS O	-22.75	-32.84	76.60	21.41
108 ARG N	-24.66	-34.00	76.40	22.61
108 ARG CA	-23.96	-35.28	76.44	25.98
108 ARG CB	-24.57	-36.18	77.53	25.00
108 ARG CG	-24.76	-35.44	78.85	19.33
108 ARG CD	-25.24	-36.32	79.99	17.89
108 ARG NE	-26.61	-36.80	79.81	10.20
108 ARG CZ	-27.00	-38.02	80.15	9.00
108 ARG NH1	-26.12	-38.88	80.68	6.62
108 ARG NH2	-28.26	-38.39	79.99	10.32
108 ARG C	-23.91	-35.98	75.08	23.86
108 ARG O	-24.38	-37.10	74.94	25.08
109 GLY N	-23.34	-35.29	74.10	23.61
109 GLY CA	-23.21	-35.84	72.76	20.68
109 GLY C	-24.30	-35.35	71.82	18.95
109 GLY O	-25.15	-34.56	72.22	19.25
110 TYR N	-24.29	-35.85	70.58	18.18
110 TYR CA	-25.27	-35.46	69.57	17.03
110 TYR CB	-24.72	-34.38	68.64	14.76
110 TYR CG	-23.48	-34.81	67.90	12.25
110 TYR CD1	-22.21	-34.48	68.37	14.76
110 TYR CE1	-21.06	-34.95	67.75	14.89
110 TYR CD2	-23.56	-35.61	66.78	12.73
110 TYR CE2	-22.41	-36.08	66.14	15.02

TABLE VII

110	TYR	CZ	-21.17	-35.75	66.64	17.33
110	TYR	OH	-20.03	-36.26	66.03	22.26
110	TYR	C	-25.70	-36.67	68.75	16.81
110	TYR	O	-25.01	-37.69	68.73	19.27
111	ARG	N	-26.83	-36.53	68.07	16.77
111	ARG	CA	-27.34	-37.57	67.19	18.25
111	ARG	CB	-28.73	-38.08	67.60	20.39
111	ARG	CG	-29.51	-38.81	66.48	21.92
111	ARG	CD	-28.94	-40.20	66.16	26.51
111	ARG	NE	-29.54	-40.85	64.98	25.17
111	ARG	CZ	-28.83	-41.49	64.03	26.40
111	ARG	NH1	-27.50	-41.55	64.12	21.95
111	ARG	NH2	-29.45	-42.10	63.02	18.73
111	ARG	C	-27.43	-36.92	65.81	20.54
111	ARG	O	-27.88	-35.77	65.69	23.20
112	GLU	N	-26.95	-37.62	64.79	17.24
112	GLU	CA	-27.01	-37.12	63.42	13.69
112	GLU	CB	-25.70	-37.34	62.69	12.60
112	GLU	CG	-24.59	-36.38	63.05	10.04
112	GLU	CD	-23.25	-36.92	62.62	11.35
112	GLU	OE1	-22.50	-36.23	61.89	10.65
112	GLU	OE2	-22.97	-38.06	63.01	14.44
112	GLU	C	-28.15	-37.85	62.72	15.47
112	GLU	O	-28.49	-38.97	63.09	17.83
113	ILE	N	-28.72	-37.25	61.70	17.43
113	ILE	CA	-29.82	-37.87	60.96	14.32
113	ILE	CB	-30.99	-36.87	60.90	13.01
113	ILE	CG2	-32.04	-37.32	59.87	11.54
113	ILE	CG1	-31.55	-36.70	62.33	10.24
113	ILE	CD1	-32.35	-35.44	62.57	7.36
113	ILE	C	-29.38	-38.34	59.57	12.75
113	ILE	O	-28.59	-37.68	58.91	11.81
114	PRO	N	-29.83	-39.53	59.13	15.44
114	PRO	CD	-30.82	-40.40	59.80	19.88
114	PRO	CA	-29.47	-40.08	57.81	15.21
114	PRO	CB	-30.54	-41.13	57.59	15.21
114	PRO	CG	-30.79	-41.66	58.96	16.85
114	PRO	C	-29.53	-39.00	56.73	18.58
114	PRO	O	-30.52	-38.27	56.64	21.69
115	GLU	N	-28.49	-38.91	55.91	17.93
115	GLU	CA	-28.45	-37.90	54.87	18.15
115	GLU	CB	-27.12	-37.95	54.11	21.41

TABLE VII

115	GLU	CG	-27.04	-39.05	53.06	28.55
115	GLU	CD	-25.73	-39.04	52.26	34.52
115	GLU	OE1	-25.24	-37.94	51.90	34.27
115	GLU	OE2	-25.21	-40.14	51.99	34.99
115	GLU	C	-29.63	-37.99	53.90	20.57
115	GLU	O	-30.10	-39.08	53.56	20.47
116	GLY	N	-30.13	-36.82	53.51	21.25
116	GLY	CA	-31.24	-36.73	52.58	19.05
116	GLY	C	-32.59	-37.14	53.12	19.97
116	GLY	O	-33.62	-36.74	52.56	24.15
117	ASN	N	-32.62	-37.87	54.23	17.37
117	ASN	CA	-33.90	-38.33	54.77	15.93
117	ASN	CB	-33.73	-39.57	55.64	10.26
117	ASN	CG	-35.03	-40.34	55.79	12.00
117	ASN	OD1	-36.12	-39.76	55.79	10.30
117	ASN	ND2	-34.92	-41.66	55.91	13.10
117	ASN	C	-34.73	-37.30	55.49	17.41
117	ASN	O	-34.57	-37.09	56.70	18.71
118	GLU	N	-35.66	-36.70	54.77	15.53
118	GLU	CA	-36.56	-35.71	55.34	15.33
118	GLU	CB	-37.27	-34.93	54.25	15.94
118	GLU	CG	-36.37	-34.00	53.46	22.20
118	GLU	CD	-37.14	-33.16	52.46	21.94
118	GLU	OE1	-37.27	-33.58	51.29	25.99
118	GLU	OE2	-37.64	-32.08	52.85	25.26
118	GLU	C	-37.57	-36.30	56.33	18.60
118	GLU	O	-38.02	-35.60	57.23	23.43
119	LYS	N	-37.93	-37.57	56.17	19.21
119	LYS	CA	-38.89	-38.21	57.08	17.16
119	LYS	CB	-39.39	-39.55	56.54	18.23
119	LYS	CG	-40.29	-39.44	55.34	23.03
119	LYS	CD	-41.48	-38.55	55.62	24.88
119	LYS	CE	-41.85	-37.77	54.36	33.17
119	LYS	NZ	-40.65	-37.07	53.78	35.51
119	LYS	C	-38.30	-38.39	58.44	13.83
119	LYS	O	-38.99	-38.27	59.45	14.48
120	ALA	N	-37.02	-38.74	58.47	11.43
120	ALA	CA	-36.30	-38.93	59.71	11.35
120	ALA	CB	-34.91	-39.44	59.43	12.94
120	ALA	C	-36.23	-37.57	60.34	14.11
120	ALA	O	-36.49	-37.41	61.53	20.36
121	LEU	N	-35.94	-36.57	59.52	14.09

TABLE VII

121 LEU CA	-35.84	-35.19	59.98	14.37
121 LEU CB	-35.35	-34.28	58.86	11.45
121 LEU CG	-35.11	-32.82	59.20	13.53
121 LEU CD1	-34.22	-32.69	60.44	17.91
121 LEU CD2	-34.49	-32.13	57.98	13.43
121 LEU C	-37.17	-34.71	60.57	14.14
121 LEU O	-37.19	-34.08	61.63	17.50
122 LYS N	-38.28	-35.01	59.90	14.51
122 LYS CA	-39.61	-34.63	60.36	14.97
122 LYS CB	-40.67	-34.97	59.32	15.25
122 LYS CG	-42.09	-34.67	59.75	15.73
122 LYS CD	-43.09	-35.54	59.00	15.63
122 LYS CE	-44.48	-35.36	59.56	22.12
122 LYS NZ	-45.45	-36.35	59.02	25.27
122 LYS C	-39.93	-35.32	61.69	17.92
122 LYS O	-40.58	-34.74	62.58	15.41
123 ARG N	-39.51	-36.57	61.80	20.19
123 ARG CA	-39.71	-37.36	63.00	24.53
123 ARG CB	-39.36	-38.82	62.76	26.04
123 ARG CG	-40.37	-39.57	61.92	29.94
123 ARG CD	-39.79	-40.87	61.39	33.27
123 ARG NE	-38.98	-41.56	62.39	38.93
123 ARG CZ	-37.67	-41.79	62.26	38.64
123 ARG NH1	-37.03	-41.37	61.18	39.92
123 ARG NH2	-37.00	-42.45	63.20	34.71
123 ARG C	-38.89	-36.77	64.14	25.64
123 ARG O	-39.33	-36.76	65.30	25.72
124 ALA N	-37.70	-36.26	63.80	23.74
124 ALA CA	-36.80	-35.64	64.77	25.05
124 ALA CB	-35.49	-35.23	64.09	22.46
124 ALA C	-37.48	-34.41	65.37	24.90
124 ALA O	-37.50	-34.23	66.59	25.58
125 VAL N	-38.02	-33.57	64.50	25.44
125 VAL CA	-38.69	-32.35	64.92	24.60
125 VAL CB	-39.08	-31.46	63.72	20.30
125 VAL CG1	-39.85	-30.23	64.19	13.27
125 VAL CG2	-37.80	-31.05	62.95	19.58
125 VAL C	-39.93	-32.66	65.73	24.17
125 VAL O	-40.19	-32.01	66.73	26.08
126 ALA N	-40.69	-33.66	65.32	25.26
126 ALA CA	-41.90	-34.00	66.05	26.85
126 ALA CB	-42.65	-35.08	65.34	27.49

TABLE VII

126	ALA	C	-41.59	-34.41	67.50	28.51
126	ALA	O	-42.22	-33.91	68.43	29.45
127	ARG	N	-40.60	-35.30	67.68	27.15
127	ARG	CA	-40.20	-35.80	69.01	26.50
127	ARG	CB	-39.52	-37.17	68.92	25.80
127	ARG	CG	-40.36	-38.31	68.39	29.17
127	ARG	CD	-41.39	-38.82	69.38	30.20
127	ARG	NE	-42.01	-40.06	68.90	31.67
127	ARG	CZ	-43.14	-40.57	69.38	31.87
127	ARG	NH1	-43.62	-41.70	68.87	32.34
127	ARG	NH2	-43.80	-39.97	70.36	33.34
127	ARG	C	-39.30	-34.88	69.83	26.63
127	ARG	O	-39.61	-34.54	70.98	29.49
128	VAL	N	-38.13	-34.58	69.27	24.07
128	VAL	CA	-37.14	-33.75	69.93	20.27
128	VAL	CB	-35.74	-33.96	69.29	17.18
128	VAL	CG1	-34.73	-33.00	69.87	16.62
128	VAL	CG2	-35.27	-35.40	69.51	16.17
128	VAL	C	-37.51	-32.28	69.92	19.91
128	VAL	O	-38.00	-31.75	70.91	21.31
129	GLY	N	-37.26	-31.63	68.79	21.40
129	GLY	CA	-37.56	-30.22	68.67	18.08
129	GLY	C	-36.62	-29.60	67.67	17.76
129	GLY	O	-36.22	-30.27	66.71	14.46
130	PRO	N	-36.25	-28.33	67.86	18.11
130	PRO	CD	-36.68	-27.44	68.96	20.59
130	PRO	CA	-35.35	-27.64	66.94	17.36
130	PRO	CB	-35.03	-26.36	67.70	17.67
130	PRO	CG	-36.33	-26.07	68.41	19.12
130	PRO	C	-34.10	-28.47	66.69	18.18
130	PRO	O	-33.43	-28.92	67.63	21.49
131	VAL	N	-33.81	-28.71	65.41	14.71
131	VAL	CA	-32.66	-29.47	64.99	10.15
131	VAL	CB	-33.09	-30.69	64.16	13.09
131	VAL	CG1	-31.88	-31.39	63.55	14.17
131	VAL	CG2	-33.88	-31.63	65.02	19.95
131	VAL	C	-31.80	-28.60	64.10	10.57
131	VAL	O	-32.33	-27.86	63.27	13.19
132	SER	N	-30.49	-28.71	64.25	7.45
132	SER	CA	-29.59	-27.93	63.42	7.72
132	SER	CB	-28.23	-27.81	64.07	9.68
132	SER	OG	-28.37	-27.45	65.44	20.96

TABLE VII

132 SER C	-29.48	-28.55	62.02	6.88
132 SER O	-29.18	-29.74	61.86	4.58
133 VAL N	-29.75	-27.75	61.00	7.92
133 VAL CA	-29.68	-28.20	59.62	6.47
133 VAL CB	-31.09	-28.35	59.00	6.27
133 VAL CG1	-31.92	-29.35	59.80	5.31
133 VAL CG2	-31.80	-27.00	58.93	2.32
133 VAL C	-28.88	-27.20	58.78	6.11
133 VAL O	-28.93	-25.99	59.01	4.92
134 ALA N	-28.09	-27.71	57.85	8.55
134 ALA CA	-27.29	-26.90	56.94	10.56
134 ALA CB	-25.90	-27.49	56.80	10.48
134 ALA C	-28.01	-26.89	55.59	11.28
134 ALA O	-28.61	-27.91	55.19	10.70
135 ILE N	-28.00	-25.75	54.91	5.87
135 ILE CA	-28.65	-25.64	53.61	9.02
135 ILE CB	-30.05	-25.04	53.75	9.82
135 ILE CG2	-30.96	-25.98	54.52	8.18
135 ILE CG1	-29.97	-23.67	54.42	7.95
135 ILE CD1	-31.24	-22.87	54.30	5.36
135 ILE C	-27.84	-24.75	52.67	10.58
135 ILE O	-26.82	-24.17	53.08	11.83
136 ASP N	-28.27	-24.67	51.41	14.26
136 ASP CA	-27.64	-23.83	50.39	12.77
136 ASP CB	-27.59	-24.54	49.03	11.56
136 ASP CG	-27.29	-23.58	47.87	11.70
136 ASP OD1	-27.82	-23.80	46.77	16.82
136 ASP OD2	-26.54	-22.61	48.06	6.89
136 ASP C	-28.44	-22.53	50.29	11.76
136 ASP O	-29.51	-22.50	49.69	12.86
137 ALA N	-27.90	-21.45	50.83	12.10
137 ALA CA	-28.63	-20.19	50.80	14.12
137 ALA CB	-28.77	-19.64	52.22	16.96
137 ALA C	-28.02	-19.14	49.87	15.39
137 ALA O	-28.27	-17.94	50.04	11.83
138 SER N	-27.20	-19.57	48.91	16.46
138 SER CA	-26.56	-18.66	47.96	16.14
138 SER CB	-25.45	-19.36	47.17	13.20
138 SER OG	-25.91	-20.60	46.65	11.80
138 SER C	-27.54	-17.97	47.02	17.22
138 SER O	-27.42	-16.77	46.74	16.85
139 LEU N	-28.50	-18.75	46.53	11.84

TABLE VII

139	LEU CA	-29.51	-18.24	45.62	10.88
139	LEU CB	-30.62	-19.27	45.41	10.28
139	LEU CG	-30.39	-20.25	44.25	7.79
139	LEU CD1	-28.98	-20.81	44.28	16.09
139	LEU CD2	-31.39	-21.35	44.31	6.66
139	LEU C	-30.07	-16.90	46.07	10.95
139	LEU O	-30.56	-16.77	47.18	10.84
140	THR N	-29.98	-15.89	45.20	12.65
140	THR CA	-30.48	-14.56	45.55	10.04
140	THR CB	-30.04	-13.47	44.54	8.74
140	THR OG1	-30.71	-13.68	43.29	16.41
140	THR CG2	-28.52	-13.50	44.33	5.90
140	THR C	-31.98	-14.51	45.76	7.53
140	THR O	-32.51	-13.48	46.16	7.86
141	SER N	-32.69	-15.60	45.48	7.62
141	SER CA	-34.13	-15.60	45.71	10.59
141	SER CB	-34.81	-16.69	44.90	7.78
141	SER OG	-34.14	-17.92	45.09	10.19
141	SER C	-34.32	-15.81	47.21	14.46
141	SER O	-35.31	-15.38	47.80	15.07
142	PHE N	-33.33	-16.47	47.81	16.29
142	PHE CA	-33.32	-16.75	49.24	18.29
142	PHE CB	-32.26	-17.80	49.57	19.91
142	PHE CG	-32.23	-18.22	51.01	19.34
142	PHE CD1	-32.83	-19.42	51.40	19.10
142	PHE CD2	-31.58	-17.44	51.96	17.86
142	PHE CE1	-32.77	-19.84	52.72	18.29
142	PHE CE2	-31.52	-17.86	53.29	16.09
142	PHE CZ	-32.12	-19.06	53.67	17.03
142	PHE C	-33.04	-15.46	49.98	18.87
142	PHE O	-33.70	-15.13	50.96	20.82
143	GLN N	-32.06	-14.71	49.48	17.89
143	GLN CA	-31.69	-13.46	50.11	17.94
143	GLN CB	-30.35	-12.98	49.56	20.86
143	GLN CG	-29.29	-14.07	49.66	27.97
143	GLN CD	-27.96	-13.66	49.06	35.25
143	GLN OE1	-27.88	-12.65	48.36	42.66
143	GLN NE2	-26.91	-14.44	49.35	32.14
143	GLN C	-32.77	-12.40	49.97	16.38
143	GLN O	-32.78	-11.43	50.72	21.06
144	PHE N	-33.71	-12.62	49.07	16.70
144	PHE CA	-34.81	-11.68	48.86	16.93

TABLE VII

144 PHE CB	-34.83	-11.16	47.42	14.35
144 PHE CG	-33.63	-10.34	47.06	9.94
144 PHE CD1	-33.23	-9.28	47.87	7.40
144 PHE CD2	-32.87	-10.63	45.94	11.47
144 PHE CE1	-32.09	-8.54	47.58	2.23
144 PHE CE2	-31.73	-9.89	45.63	11.16
144 PHE CZ	-31.34	-8.85	46.45	5.01
144 PHE C	-36.15	-12.29	49.26	19.07
144 PHE O	-37.21	-11.75	48.94	23.82
145 TYR N	-36.10	-13.42	49.95	21.54
145 TYR CA	-37.31	-14.10	50.39	20.66
145 TYR CB	-36.98	-15.43	51.09	19.50
145 TYR CG	-38.13	-16.04	51.85	20.41
145 TYR CD1	-38.96	-16.98	51.25	22.31
145 TYR CE1	-40.05	-17.51	51.93	23.37
145 TYR CD2	-38.43	-15.64	53.15	19.98
145 TYR CE2	-39.52	-16.16	53.84	20.51
145 TYR CZ	-40.33	-17.09	53.22	22.20
145 TYR OH	-41.42	-17.60	53.89	24.45
145 TYR C	-38.13	-13.18	51.31	19.31
145 TYR O	-37.57	-12.41	52.09	16.29
146 SER N	-39.44	-13.29	51.23	19.16
146 SER CA	-40.31	-12.46	52.05	18.38
146 SER CB	-40.69	-11.17	51.33	21.74
146 SER OG	-41.24	-11.45	50.05	25.62
146 SER C	-41.55	-13.21	52.52	17.33
146 SER O	-41.87	-13.19	53.70	17.00
147 LYS N	-42.21	-13.90	51.60	15.30
147 LYS CA	-43.42	-14.63	51.94	16.47
147 LYS CB	-44.65	-13.72	51.85	21.13
147 LYS CG	-45.98	-14.43	52.13	26.90
147 LYS CD	-47.15	-13.75	51.41	31.88
147 LYS CE	-48.38	-14.69	51.35	38.13
147 LYS NZ	-49.45	-14.23	50.41	36.35
147 LYS C	-43.61	-15.88	51.09	16.19
147 LYS O	-43.21	-15.91	49.92	18.85
148 GLY N	-44.20	-16.91	51.69	14.07
148 GLY CA	-44.47	-18.14	50.98	13.24
148 GLY C	-43.46	-19.26	51.17	12.23
148 GLY O	-42.39	-19.05	51.74	11.43
149 VAL N	-43.82	-20.45	50.71	9.32
149 VAL CA	-42.95	-21.61	50.81	8.20

TABLE VII

149 VAL CB	-43.70	-22.96	50.60	5.83
149 VAL CG1	-42.72	-24.11	50.73	2.00
149 VAL CG2	-44.82	-23.12	51.61	4.34
149 VAL C	-41.92	-21.43	49.70	11.54
149 VAL O	-42.25	-21.45	48.50	12.48
150 TYR N	-40.68	-21.21	50.13	12.91
150 TYR CA	-39.55	-21.02	49.24	10.42
150 TYR CB	-38.33	-20.58	50.03	4.78
150 TYR CG	-37.10	-20.42	49.19	8.23
150 TYR CD1	-36.83	-19.21	48.55	10.09
150 TYR CE1	-35.68	-19.06	47.77	11.54
150 TYR CD2	-36.21	-21.47	49.02	8.80
150 TYR CE2	-35.07	-21.33	48.24	9.65
150 TYR CZ	-34.81	-20.13	47.62	10.30
150 TYR OH	-33.67	-19.97	46.88	18.73
150 TYR C	-39.27	-22.30	48.46	14.00
150 TYR O	-39.45	-23.40	48.96	16.63
151 TYR N	-38.79	-22.13	47.24	15.66
151 TYR CA	-38.48	-23.25	46.37	17.45
151 TYR CB	-39.74	-24.04	46.01	21.54
151 TYR CG	-39.53	-25.25	45.13	23.93
151 TYR CD1	-38.93	-26.42	45.64	28.17
151 TYR CE1	-38.74	-27.54	44.83	29.69
151 TYR CD2	-39.94	-25.25	43.80	26.78
151 TYR CE2	-39.76	-26.36	42.99	29.59
151 TYR CZ	-39.16	-27.50	43.51	32.44
151 TYR OH	-38.99	-28.60	42.70	37.61
151 TYR C	-37.85	-22.60	45.15	18.03
151 TYR O	-38.32	-21.56	44.68	16.75
152 ASP N	-36.76	-23.17	44.68	19.75
152 ASP CA	-36.05	-22.64	43.52	21.69
152 ASP CB	-35.07	-21.53	43.91	21.35
152 ASP CG	-34.48	-20.80	42.70	22.73
152 ASP OD1	-34.58	-19.56	42.63	20.20
152 ASP OD2	-33.90	-21.46	41.82	23.61
152 ASP C	-35.33	-23.85	42.96	25.58
152 ASP O	-34.67	-24.57	43.72	28.85
153 GLU N	-35.50	-24.09	41.66	26.65
153 GLU CA	-34.86	-25.25	41.03	26.63
153 GLU CB	-35.52	-25.57	39.69	30.19
153 GLU CG	-36.09	-24.38	38.92	34.99
153 GLU CD	-35.04	-23.61	38.15	37.99

TABLE VII

153	GLU	OE1	-34.95	-22.38	38.34	40.14
153	GLU	OE2	-34.31	-24.24	37.34	40.23
153	GLU	C	-33.34	-25.20	40.91	24.39
153	GLU	O	-32.71	-26.22	40.70	23.54
154	SER	N	-32.75	-24.02	41.11	23.15
154	SER	CA	-31.30	-23.83	41.04	25.05
154	SER	CB	-30.95	-22.35	40.85	24.11
154	SER	OG	-31.81	-21.71	39.91	26.07
154	SER	C	-30.53	-24.38	42.26	25.62
154	SER	O	-29.37	-24.78	42.15	26.42
155	CYS	N	-31.19	-24.33	43.43	24.27
155	CYS	CA	-30.63	-24.77	44.71	19.73
155	CYS	C	-29.88	-26.08	44.59	17.05
155	CYS	O	-30.44	-27.08	44.16	14.86
155	CYS	CB	-31.72	-24.87	45.79	20.11
155	CYS	SG	-31.27	-24.12	47.40	19.94
156	ASN	N	-28.61	-26.07	44.99	19.11
156	ASN	CA	-27.76	-27.26	44.92	21.62
156	ASN	CB	-26.37	-26.87	44.41	19.84
156	ASN	CG	-25.47	-28.06	44.20	20.15
156	ASN	OD1	-25.86	-29.20	44.44	15.60
156	ASN	ND2	-24.23	-27.80	43.77	19.95
156	ASN	C	-27.67	-28.05	46.24	22.71
156	ASN	O	-27.08	-27.58	47.21	23.56
157	SER	N	-28.20	-29.28	46.23	22.09
157	SER	CA	-28.22	-30.17	47.40	16.83
157	SER	CB	-28.93	-31.49	47.06	14.81
157	SER	OG	-30.26	-31.26	46.66	19.44
157	SER	C	-26.86	-30.49	48.02	17.43
157	SER	O	-26.78	-31.10	49.10	16.02
158	ASP	N	-25.79	-30.19	47.30	17.73
158	ASP	CA	-24.46	-30.46	47.80	20.40
158	ASP	CB	-23.70	-31.42	46.88	24.69
158	ASP	CG	-24.27	-32.82	46.89	27.15
158	ASP	OD1	-24.93	-33.19	45.88	26.00
158	ASP	OD2	-24.08	-33.55	47.90	26.52
158	ASP	C	-23.68	-29.19	48.00	20.27
158	ASP	O	-22.46	-29.22	48.16	20.24
159	ASN	N	-24.39	-28.07	47.97	17.11
159	ASN	CA	-23.72	-26.81	48.19	16.88
159	ASN	CB	-24.01	-25.79	47.10	18.24
159	ASN	CG	-23.00	-24.66	47.10	21.17

TABLE VII

159 ASN OD1	-21.83	-24.86	47.42	16.98
159 ASN ND2	-23.46	-23.46	46.75	22.38
159 ASN C	-24.12	-26.28	49.55	17.56
159 ASN O	-24.64	-25.17	49.67	19.13
160 LEU N	-23.93	-27.12	50.57	12.99
160 LEU CA	-24.23	-26.73	51.94	8.24
160 LEU CB	-24.00	-27.89	52.89	4.68
160 LEU CG	-25.09	-28.95	53.11	5.66
160 LEU CD1	-25.96	-29.16	51.89	3.96
160 LEU CD2	-24.43	-30.24	53.54	6.24
160 LEU C	-23.28	-25.58	52.23	8.29
160 LEU O	-22.07	-25.75	52.11	8.75
161 ASN N	-23.83	-24.41	52.54	9.39
161 ASN CA	-23.02	-23.23	52.83	10.51
161 ASN CB	-22.74	-22.43	51.56	14.18
161 ASN CG	-24.01	-22.01	50.85	10.89
161 ASN OD1	-24.80	-21.22	51.35	14.49
161 ASN ND2	-24.21	-22.56	49.67	16.31
161 ASN C	-23.56	-22.29	53.92	12.43
161 ASN O	-23.02	-21.20	54.14	13.86
162 HIS N	-24.62	-22.69	54.60	11.27
162 HIS CA	-25.19	-21.85	55.64	10.37
162 HIS CB	-26.13	-20.82	55.00	5.69
162 HIS CG	-26.80	-19.89	55.96	6.06
162 HIS CD2	-28.10	-19.79	56.33	6.15
162 HIS ND1	-26.14	-18.85	56.61	11.02
162 HIS CE1	-27.01	-18.16	57.33	5.27
162 HIS NE2	-28.20	-18.71	57.17	6.68
162 HIS C	-25.92	-22.76	56.61	11.99
162 HIS O	-26.68	-23.63	56.20	15.71
163 ALA N	-25.59	-22.65	57.89	14.09
163 ALA CA	-26.22	-23.48	58.91	10.89
163 ALA CB	-25.26	-23.79	60.01	12.33
163 ALA C	-27.38	-22.67	59.43	8.08
163 ALA O	-27.24	-21.48	59.69	7.93
164 VAL N	-28.52	-23.33	59.61	8.61
164 VAL CA	-29.73	-22.67	60.06	9.19
164 VAL CB	-30.58	-22.36	58.82	13.42
164 VAL CG1	-31.55	-23.51	58.50	8.48
164 VAL CG2	-31.22	-21.00	58.93	12.71
164 VAL C	-30.45	-23.60	61.06	9.94
164 VAL O	-29.95	-24.69	61.35	11.85

TABLE VII

165 LEU N	-31.59	-23.20	61.61	5.74
165 LEU CA	-32.29	-24.07	62.58	6.61
165 LEU CB	-32.27	-23.43	63.97	3.31
165 LEU CG	-32.85	-24.20	65.15	2.00
165 LEU CD1	-31.81	-25.14	65.69	3.91
165 LEU CD2	-33.27	-23.20	66.22	3.66
165 LEU C	-33.71	-24.47	62.20	8.12
165 LEU O	-34.52	-23.62	61.80	12.38
166 ALA N	-34.04	-25.75	62.36	6.76
166 ALA CA	-35.37	-26.25	62.02	6.92
166 ALA CB	-35.28	-27.67	61.50	5.38
166 ALA C	-36.29	-26.20	63.24	9.15
166 ALA O	-36.23	-27.07	64.10	12.12
167 VAL N	-37.15	-25.19	63.30	10.50
167 VAL CA	-38.06	-25.06	64.42	10.11
167 VAL CB	-38.16	-23.60	64.93	9.38
167 VAL CG1	-36.79	-23.07	65.35	2.39
167 VAL CG2	-38.82	-22.71	63.88	7.39
167 VAL C	-39.47	-25.56	64.11	10.07
167 VAL O	-40.44	-25.13	64.73	12.94
168 GLY N	-39.60	-26.47	63.16	9.76
168 GLY CA	-40.93	-26.97	62.85	7.51
168 GLY C	-41.09	-27.55	61.46	8.86
168 GLY O	-40.11	-27.88	60.80	7.84
169 TYR N	-42.34	-27.71	61.06	10.03
169 TYR CA	-42.70	-28.24	59.76	12.55
169 TYR CB	-42.20	-29.67	59.56	12.27
169 TYR CG	-42.79	-30.71	60.51	12.03
169 TYR CD1	-44.13	-31.06	60.43	9.03
169 TYR CE1	-44.67	-32.02	61.26	9.87
169 TYR CD2	-42.00	-31.35	61.45	11.40
169 TYR CE2	-42.54	-32.31	62.30	8.77
169 TYR CZ	-43.87	-32.64	62.19	6.67
169 TYR OH	-44.45	-33.58	63.00	8.74
169 TYR C	-44.21	-28.15	59.68	15.32
169 TYR O	-44.88	-28.12	60.72	19.66
170 GLY N	-44.77	-28.10	58.47	15.75
170 GLY CA	-46.21	-28.00	58.36	13.53
170 GLY C	-46.70	-28.03	56.94	14.99
170 GLY O	-46.13	-28.72	56.09	14.31
171 ILE N	-47.70	-27.21	56.66	17.47
171 ILE CA	-48.28	-27.14	55.33	23.06

TABLE VII

171 ILE CB	-49.37	-28.23	55.17	25.40
171 ILE CG2	-50.56	-27.93	56.06	30.02
171 ILE CG1	-49.86	-28.31	53.73	33.16
171 ILE CD1	-49.86	-29.73	53.19	37.53
171 ILE C	-48.86	-25.75	55.07	21.85
171 ILE O	-49.14	-25.02	56.01	26.83
172 GLN N	-48.95	-25.33	53.81	24.21
172 GLN CA	-49.52	-24.03	53.46	24.63
172 GLN CB	-48.53	-22.88	53.66	22.98
172 GLN CG	-49.13	-21.50	53.34	24.04
172 GLN CD	-48.15	-20.35	53.49	25.53
172 GLN OE1	-47.37	-20.30	54.45	30.09
172 GLN NE2	-48.17	-19.42	52.55	28.42
172 GLN C	-50.02	-24.03	52.02	25.83
172 GLN O	-49.24	-24.28	51.09	28.71
173 LYS N	-51.32	-23.80	51.83	23.80
173 LYS CA	-51.91	-23.78	50.49	22.33
173 LYS CB	-51.58	-22.46	49.78	22.26
173 LYS CG	-52.35	-21.23	50.29	26.56
173 LYS CD	-53.81	-21.23	49.80	30.52
173 LYS CE	-54.48	-19.85	49.89	29.44
173 LYS NZ	-54.64	-19.30	51.27	28.52
173 LYS C	-51.45	-24.98	49.66	21.89
173 LYS O	-51.02	-24.84	48.52	22.66
174 GLY N	-51.49	-26.16	50.27	21.87
174 GLY CA	-51.08	-27.38	49.61	20.01
174 GLY C	-49.59	-27.70	49.71	19.12
174 GLY O	-49.18	-28.85	49.49	14.08
175 ASN N	-48.79	-26.71	50.06	19.25
175 ASN CA	-47.34	-26.90	50.16	22.03
175 ASN CB	-46.59	-25.65	49.70	23.43
175 ASN CG	-47.13	-25.08	48.40	26.87
175 ASN OD1	-46.80	-25.56	47.31	24.31
175 ASN ND2	-47.96	-24.04	48.52	27.46
175 ASN C	-46.85	-27.30	51.56	22.36
175 ASN O	-46.95	-26.52	52.51	22.73
176 LYS N	-46.34	-28.52	51.69	18.82
176 LYS CA	-45.79	-28.98	52.95	18.15
176 LYS CB	-45.64	-30.50	52.97	19.27
176 LYS CG	-46.95	-31.32	53.07	21.41
176 LYS CD	-46.63	-32.84	52.96	17.01
176 LYS CE	-47.83	-33.72	53.27	21.32

TABLE VII

176 LYS NZ	-48.07	-33.97	54.73	17.44
176 LYS C	-44.42	-28.30	53.03	20.70
176 LYS O	-43.56	-28.53	52.17	21.72
177 HIS N	-44.19	-27.51	54.08	18.91
177 HIS CA	-42.93	-26.78	54.26	13.73
177 HIS CB	-43.18	-25.28	54.19	16.90
177 HIS CG	-44.04	-24.76	55.30	17.13
177 HIS CD2	-43.77	-24.55	56.62	20.36
177 HIS ND1	-45.37	-24.39	55.13	20.15
177 HIS CE1	-45.87	-23.99	56.28	21.57
177 HIS NE2	-44.92	-24.08	57.20	21.14
177 HIS C	-42.20	-27.08	55.56	13.57
177 HIS O	-42.71	-27.80	56.42	15.98
178 TRP N	-41.05	-26.45	55.74	11.27
178 TRP CA	-40.27	-26.56	56.97	10.08
178 TRP CB	-38.80	-26.95	56.72	13.29
178 TRP CG	-38.53	-28.36	56.29	9.82
178 TRP CD2	-38.48	-29.53	57.12	13.57
178 TRP CE2	-38.10	-30.61	56.30	13.92
178 TRP CE3	-38.73	-29.77	58.48	15.49
178 TRP CD1	-38.19	-28.77	55.04	12.10
178 TRP NE1	-37.93	-30.12	55.03	13.58
178 TRP CZ2	-37.95	-31.92	56.79	14.49
178 TRP CZ3	-38.58	-31.07	58.97	16.39
178 TRP CH2	-38.19	-32.13	58.12	16.81
178 TRP C	-40.31	-25.13	57.51	10.66
178 TRP O	-40.55	-24.19	56.75	11.76
179 ILE N	-40.13	-24.95	58.82	11.11
179 ILE CA	-40.11	-23.61	59.41	9.30
179 ILE CB	-40.99	-23.50	60.66	11.02
179 ILE CG2	-40.96	-22.10	61.21	3.09
179 ILE CG1	-42.44	-23.88	60.33	9.87
179 ILE CD1	-43.38	-23.79	61.52	10.20
179 ILE C	-38.66	-23.46	59.79	10.91
179 ILE O	-38.13	-24.27	60.55	13.14
180 ILE N	-38.01	-22.45	59.23	12.47
180 ILE CA	-36.60	-22.25	59.48	10.39
180 ILE CB	-35.84	-22.35	58.14	4.50
180 ILE CG2	-34.41	-21.90	58.27	4.54
180 ILE CG1	-35.91	-23.78	57.61	6.63
180 ILE CD1	-35.21	-24.85	58.48	10.08
180 ILE C	-36.27	-20.95	60.18	12.35

TABLE VII

180 ILE O	-36.73	-19.88	59.76	18.36
181 LYS N	-35.50	-21.05	61.27	9.02
181 LYS CA	-35.06	-19.88	62.03	6.93
181 LYS CB	-34.92	-20.19	63.52	8.20
181 LYS CG	-34.55	-18.99	64.39	4.18
181 LYS CD	-34.21	-19.41	65.80	5.00
181 LYS CE	-33.83	-18.23	66.69	2.00
181 LYS NZ	-33.38	-18.69	68.03	2.00
181 LYS C	-33.71	-19.45	61.47	6.56
181 LYS O	-32.76	-20.23	61.51	9.50
182 ASN N	-33.63	-18.25	60.93	6.31
182 ASN CA	-32.38	-17.79	60.36	7.51
182 ASN CB	-32.62	-17.18	58.97	12.34
182 ASN CG	-31.37	-17.16	58.12	13.66
182 ASN OD1	-30.38	-17.83	58.43	13.80
182 ASN ND2	-31.40	-16.41	57.03	14.20
182 ASN C	-31.67	-16.80	61.27	8.95
182 ASN O	-32.29	-16.18	62.12	9.35
183 SER N	-30.37	-16.65	61.07	12.23
183 SER CA	-29.55	-15.74	61.87	12.33
183 SER CB	-28.41	-16.50	62.54	11.14
183 SER OG	-27.51	-17.06	61.60	2.83
183 SER C	-29.03	-14.56	61.05	17.18
183 SER O	-27.84	-14.23	61.12	14.11
184 TRP N	-29.92	-13.92	60.30	20.03
184 TRP CA	-29.59	-12.77	59.45	17.75
184 TRP CB	-29.94	-13.03	57.99	17.44
184 TRP CG	-28.96	-13.87	57.26	11.74
184 TRP CD2	-29.09	-14.40	55.93	10.49
184 TRP CE2	-27.91	-15.11	55.65	11.82
184 TRP CE3	-30.09	-14.34	54.96	7.76
184 TRP CD1	-27.75	-14.27	57.71	13.64
184 TRP NE1	-27.11	-15.01	56.76	18.22
184 TRP CZ2	-27.70	-15.76	54.44	8.06
184 TRP CZ3	-29.88	-14.99	53.75	8.86
184 TRP CH2	-28.70	-15.69	53.50	6.44
184 TRP C	-30.30	-11.51	59.91	18.70
184 TRP O	-30.21	-10.47	59.27	18.61
185 GLY N	-31.05	-11.62	61.01	19.92
185 GLY CA	-31.75	-10.48	61.55	17.99
185 GLY C	-33.25	-10.62	61.47	21.34
185 GLY O	-33.78	-11.41	60.68	24.20

TABLE VII

186 GLU N	-33.94	-9.85	62.30	25.86
186 GLU CA	-35.39	-9.85	62.34	28.63
186 GLU CB	-35.92	-9.06	63.55	33.72
186 GLU CG	-37.35	-9.41	64.01	33.62
186 GLU CD	-37.39	-10.59	64.97	33.61
186 GLU OE1	-36.64	-10.57	65.96	35.89
186 GLU OE2	-38.18	-11.54	64.74	33.82
186 GLU C	-35.93	-9.26	61.04	27.44
186 GLU O	-37.08	-9.48	60.68	29.63
187 ASN N	-35.09	-8.50	60.33	28.18
187 ASN CA	-35.54	-7.88	59.08	30.53
187 ASN CB	-35.10	-6.41	58.99	33.02
187 ASN CG	-36.04	-5.57	58.12	36.45
187 ASN OD1	-35.65	-4.51	57.62	41.13
187 ASN ND2	-37.28	-6.03	57.95	34.46
187 ASN C	-35.20	-8.65	57.79	29.17
187 ASN O	-35.12	-8.08	56.69	26.38
188 TRP N	-34.95	-9.94	57.93	26.78
188 TRP CA	-34.69	-10.76	56.76	22.32
188 TRP CB	-33.39	-11.54	56.84	20.90
188 TRP CG	-33.28	-12.47	55.69	18.19
188 TRP CD2	-33.78	-13.82	55.64	20.16
188 TRP CE2	-33.53	-14.30	54.34	16.93
188 TRP CE3	-34.43	-14.65	56.56	15.73
188 TRP CD1	-32.75	-12.21	54.46	12.09
188 TRP NE1	-32.90	-13.31	53.64	17.84
188 TRP CZ2	-33.90	-15.58	53.94	18.81
188 TRP CZ3	-34.79	-15.92	56.17	18.58
188 TRP CH2	-34.53	-16.38	54.87	19.87
188 TRP C	-35.87	-11.70	56.68	21.57
188 TRP O	-36.40	-12.11	57.72	19.48
189 GLY N	-36.28	-12.04	55.46	22.26
189 GLY CA	-37.41	-12.93	55.26	19.03
189 GLY C	-38.59	-12.53	56.12	16.83
189 GLY O	-38.70	-11.37	56.51	16.64
190 ASN N	-39.44	-13.48	56.47	19.64
190 ASN CA	-40.60	-13.17	57.30	21.04
190 ASN CB	-41.76	-14.13	57.02	18.69
190 ASN CG	-43.09	-13.58	57.49	20.80
190 ASN OD1	-43.14	-12.58	58.20	25.63
190 ASN ND2	-44.18	-14.23	57.09	16.08
190 ASN C	-40.20	-13.18	58.78	20.26

TABLE VII

190 ASN O	-40.08	-14.23	59.39	21.80
191 LYS N	-39.91	-11.99	59.31	19.09
191 LYS CA	-39.51	-11.81	60.71	17.89
191 LYS CB	-40.69	-11.99	61.66	19.60
191 LYS CG	-41.88	-11.07	61.39	20.04
191 LYS CD	-43.02	-11.37	62.36	17.35
191 LYS CE	-44.34	-10.84	61.84	16.88
191 LYS NZ	-45.47	-11.13	62.77	17.42
191 LYS C	-38.33	-12.71	61.12	14.97
191 LYS O	-38.28	-13.22	62.23	11.80
192 GLY N	-37.38	-12.87	60.20	16.54
192 GLY CA	-36.20	-13.67	60.47	10.79
192 GLY C	-36.40	-15.14	60.19	12.10
192 GLY O	-35.53	-15.94	60.52	14.29
193 TYR N	-37.53	-15.50	59.59	15.02
193 TYR CA	-37.82	-16.91	59.26	15.85
193 TYR CB	-39.02	-17.45	60.08	19.04
193 TYR CG	-38.75	-17.68	61.55	20.49
193 TYR CD1	-38.79	-16.64	62.45	23.39
193 TYR CE1	-38.52	-16.84	63.79	24.79
193 TYR CD2	-38.43	-18.95	62.02	21.17
193 TYR CE2	-38.15	-19.17	63.36	22.23
193 TYR CZ	-38.19	-18.11	64.24	24.79
193 TYR OH	-37.88	-18.29	65.56	25.50
193 TYR C	-38.11	-17.13	57.77	14.84
193 TYR O	-38.58	-16.22	57.07	11.51
194 ILE N	-37.90	-18.36	57.33	16.12
194 ILE CA	-38.16	-18.78	55.96	14.70
194 ILE CB	-36.84	-18.88	55.15	17.12
194 ILE CG2	-35.85	-19.82	55.81	13.78
194 ILE CG1	-37.11	-19.29	53.70	15.67
194 ILE CD1	-35.97	-18.96	52.77	13.44
194 ILE C	-38.92	-20.12	55.97	12.70
194 ILE O	-38.59	-21.02	56.73	11.58
195 LEU N	-39.99	-20.21	55.18	12.52
195 LEU CA	-40.79	-21.43	55.09	12.23
195 LEU CB	-42.27	-21.12	54.93	12.99
195 LEU CG	-42.88	-20.23	55.99	16.19
195 LEU CD1	-44.36	-20.05	55.68	16.70
195 LEU CD2	-42.69	-20.87	57.36	17.95
195 LEU C	-40.36	-22.30	53.93	10.25
195 LEU O	-41.15	-22.59	53.05	15.85

TABLE VII

196 MET N	-39.12	-22.76	53.96	9.10
196 MET CA	-38.58	-23.59	52.89	9.39
196 MET CB	-37.15	-23.99	53.20	8.97
196 MET CG	-36.23	-22.80	53.29	8.78
196 MET SD	-34.62	-23.28	53.80	18.24
196 MET CE	-33.88	-23.71	52.24	8.14
196 MET C	-39.43	-24.79	52.52	10.25
196 MET O	-40.21	-25.27	53.33	13.91
197 ALA N	-39.26	-25.28	51.30	11.72
197 ALA CA	-40.03	-26.42	50.82	12.43
197 ALA CB	-39.92	-26.52	49.30	7.27
197 ALA C	-39.62	-27.73	51.49	13.38
197 ALA O	-38.45	-27.92	51.85	11.55
198 ARG N	-40.58	-28.64	51.65	11.95
198 ARG CA	-40.38	-29.92	52.30	13.06
198 ARG CB	-41.05	-29.94	53.69	14.09
198 ARG CG	-41.05	-31.27	54.39	5.88
198 ARG CD	-41.44	-31.09	55.84	6.02
198 ARG NE	-42.82	-30.68	56.02	3.48
198 ARG CZ	-43.85	-31.52	56.05	6.84
198 ARG NH1	-43.64	-32.82	55.89	2.00
198 ARG NH2	-45.07	-31.08	56.35	2.52
198 ARG C	-40.94	-31.02	51.43	12.96
198 ARG O	-41.97	-30.84	50.78	15.58
199 ASN N	-40.29	-32.18	51.47	12.90
199 ASN CA	-40.66	-33.34	50.66	13.45
199 ASN CB	-42.17	-33.57	50.63	17.26
199 ASN CG	-42.69	-34.17	51.91	22.47
199 ASN OD1	-42.08	-35.09	52.47	20.71
199 ASN ND2	-43.83	-33.68	52.36	26.83
199 ASN C	-40.12	-33.20	49.24	12.34
199 ASN O	-39.63	-34.18	48.69	12.85
200 LYS N	-40.22	-32.00	48.68	10.89
200 LYS CA	-39.73	-31.64	47.34	8.22
200 LYS CB	-39.86	-30.13	47.11	8.55
200 LYS CG	-41.26	-29.57	47.04	5.90
200 LYS CD	-41.97	-30.04	45.79	9.80
200 LYS CE	-43.07	-29.09	45.40	9.34
200 LYS NZ	-42.51	-27.88	44.72	10.27
200 LYS C	-38.29	-32.09	47.02	7.56
200 LYS O	-37.43	-31.27	46.71	5.62
201 ASN N	-38.05	-33.39	47.07	9.28

TABLE VII

201 ASN CA	-36.76	-33.99	46.79	10.44
201 ASN CB	-36.58	-34.11	45.28	12.24
201 ASN CG	-37.80	-34.72	44.61	16.00
201 ASN OD1	-38.18	-35.86	44.91	12.64
201 ASN ND2	-38.47	-33.93	43.78	14.00
201 ASN C	-35.55	-33.38	47.47	10.11
201 ASN O	-34.60	-32.95	46.82	11.93
202 ASN N	-35.59	-33.36	48.80	11.90
202 ASN CA	-34.50	-32.83	49.61	9.85
202 ASN CB	-33.31	-33.79	49.55	13.31
202 ASN CG	-32.38	-33.63	50.72	13.23
202 ASN OD1	-32.82	-33.40	51.84	16.24
202 ASN ND2	-31.09	-33.81	50.47	7.73
202 ASN C	-34.09	-31.43	49.19	10.35
202 ASN O	-32.90	-31.12	49.17	13.84
203 ALA N	-35.05	-30.59	48.88	15.00
203 ALA H	-35.55	-31.01	49.01	15.00
203 ALA CA	-34.83	-29.22	48.41	15.00
203 ALA CB	-35.54	-28.63	48.10	15.00
203 ALA C	-33.66	-28.58	49.16	15.00
203 ALA O	-33.48	-28.72	50.36	18.81
204 CYS N	-32.82	-27.85	48.40	16.60
204 CYS CA	-31.68	-27.12	48.94	13.11
204 CYS C	-30.69	-27.92	49.78	13.70
204 CYS O	-29.77	-27.35	50.36	13.59
204 CYS CB	-32.14	-25.88	49.70	11.09
204 CYS SG	-32.81	-24.55	48.65	21.00
205 GLY N	-30.86	-29.23	49.82	15.46
205 GLY CA	-29.96	-30.07	50.60	17.31
205 GLY C	-30.16	-29.87	52.09	18.03
205 GLY O	-29.21	-29.94	52.87	16.28
206 ILE N	-31.42	-29.72	52.49	18.33
206 ILE CA	-31.76	-29.48	53.88	18.94
206 ILE CB	-33.23	-28.93	54.04	19.06
206 ILE CG2	-34.22	-29.85	53.34	18.93
206 ILE CG1	-33.59	-28.78	55.52	14.65
206 ILE CD1	-34.76	-27.88	55.75	16.36
206 ILE C	-31.52	-30.66	54.82	21.37
206 ILE O	-31.03	-30.47	55.94	21.08
207 ALA N	-31.79	-31.88	54.34	20.23
207 ALA CA	-31.63	-33.08	55.16	19.58
207 ALA CB	-32.79	-34.05	54.92	20.40

TABLE VII

207	ALA C	-30.29	-33.82	55.03	17.00
207	ALA O	-30.18	-34.98	55.38	15.14
208	ASN N	-29.26	-33.13	54.55	17.17
208	ASN CA	-27.97	-33.79	54.42	16.44
208	ASN CB	-27.26	-33.40	53.11	16.56
208	ASN CG	-27.95	-33.93	51.86	12.14
208	ASN OD1	-28.79	-34.83	51.91	6.67
208	ASN ND2	-27.58	-33.36	50.72	12.22
208	ASN C	-27.01	-33.56	55.59	16.20
208	ASN O	-26.14	-34.39	55.83	19.88
209	LEU N	-27.14	-32.44	56.30	11.98
209	LEU CA	-26.22	-32.16	57.40	12.42
209	LEU CB	-25.19	-31.10	56.96	11.33
209	LEU CG	-23.81	-31.03	57.61	6.60
209	LEU CD1	-23.24	-32.42	57.81	6.26
209	LEU CD2	-22.89	-30.23	56.73	6.70
209	LEU C	-26.87	-31.77	58.73	14.26
209	LEU O	-26.32	-30.96	59.48	15.18
210	ALA N	-27.99	-32.44	59.08	15.00
210	ALA H	-28.41	-32.84	58.30	15.00
210	ALA CA	-28.76	-32.10	60.27	15.00
210	ALA CB	-30.25	-32.37	60.06	15.00
210	ALA C	-28.31	-32.97	61.45	15.00
210	ALA O	-28.07	-34.16	61.40	11.82
211	SER N	-28.32	-32.32	62.66	12.69
211	SER CA	-27.97	-33.00	63.90	11.35
211	SER CB	-26.47	-33.22	64.03	10.79
211	SER OG	-25.80	-32.01	64.32	5.14
211	SER C	-28.50	-32.25	65.11	11.89
211	SER O	-28.51	-31.01	65.14	11.91
212	PHE N	-28.97	-32.99	66.09	12.57
212	PHE CA	-29.47	-32.38	67.31	11.64
212	PHE CB	-30.95	-32.69	67.51	12.77
212	PHE CG	-31.27	-34.12	67.44	11.84
212	PHE CD1	-31.61	-34.70	66.24	10.42
212	PHE CD2	-31.23	-34.91	68.58	14.45
212	PHE CE1	-31.91	-36.03	66.17	16.06
212	PHE CE2	-31.53	-36.24	68.53	15.41
212	PHE CZ	-31.87	-36.81	67.32	16.55
212	PHE C	-28.61	-32.83	68.48	12.10
212	PHE O	-27.91	-33.85	68.41	12.03
213	PRO N	-28.60	-32.05	69.57	12.99

TABLE VII

213	PRO	CD	-29.24	-30.73	69.77	10.69
213	PRO	CA	-27.79	-32.41	70.74	12.29
213	PRO	CB	-27.41	-31.05	71.29	11.67
213	PRO	CG	-28.70	-30.29	71.12	14.62
213	PRO	C	-28.56	-33.23	71.75	12.17
213	PRO	O	-29.78	-33.11	71.88	2.00
214	LYS	N	-27.82	-34.09	72.45	14.45
214	LYS	CA	-28.39	-34.94	73.50	19.77
214	LYS	CB	-27.80	-36.34	73.46	20.65
214	LYS	CG	-28.06	-37.08	72.17	24.16
214	LYS	CD	-27.54	-38.52	72.24	29.93
214	LYS	CE	-26.02	-38.57	72.40	33.14
214	LYS	NZ	-25.49	-39.97	72.44	35.37
214	LYS	C	-28.15	-34.26	74.84	21.45
214	LYS	O	-27.02	-33.92	75.20	16.74
215	MET	N	-29.23	-34.05	75.57	22.65
215	MET	CA	-29.16	-33.38	76.85	25.38
215	MET	CB	-30.04	-32.13	76.79	27.81
215	MET	CG	-29.77	-31.09	77.85	26.22
215	MET	SD	-30.44	-29.54	77.29	25.84
215	MET	CE	-28.92	-28.76	76.63	23.17
215	MET	C	-29.56	-34.30	77.99	25.33
215	MET	OT1	-28.65	-34.77	78.71	27.00
215	MET	OT2	-30.77	-34.58	78.12	23.48
216	HOH	OH2	-31.11	-16.42	65.02	14.43
217	HOH	OH2	-29.30	-20.25	62.17	18.73
218	HOH	OH2	-10.67	-12.22	63.70	43.10
219	HOH	OH2	-16.45	-12.20	72.96	5.87
220	HOH	OH2	-35.12	-23.55	69.64	9.44
221	HOH	OH2	-24.01	-30.97	61.16	4.73
222	HOH	OH2	-13.01	-8.39	61.94	32.49
223	HOH	OH2	-14.66	-21.66	66.41	2.00
224	HOH	OH2	-43.65	-26.52	48.92	29.00
225	HOH	OH2	-45.60	-35.43	55.56	13.84
226	HOH	OH2	-40.92	-17.45	68.90	12.03
227	HOH	OH2	-43.72	-25.26	44.65	38.82
228	HOH	OH2	-24.12	-5.83	68.94	43.50
229	HOH	OH2	-30.71	-18.60	67.86	32.89
230	HOH	OH2	-35.05	-26.71	51.39	30.11
231	HOH	OH2	-36.74	-24.80	49.94	8.69
232	HOH	OH2	-46.77	-33.25	57.36	12.67
233	HOH	OH2	-28.91	-10.19	75.44	15.32

TABLE VII

234	HOH	OH2	-36.31	-14.76	75.60	16.14
235	HOH	OH2	-16.18	-4.92	68.62	27.92
236	HOH	OH2	-16.52	-8.98	75.02	28.63
237	HOH	OH2	-10.50	-18.37	70.18	39.29
238	HOH	OH2	-9.29	-19.89	78.20	29.36
239	HOH	OH2	-45.95	-16.45	54.42	32.47
240	HOH	OH2	-33.98	-29.86	44.88	32.74
241	HOH	OH2	-36.55	-38.18	52.42	11.87
242	HOH	OH2	-41.73	-34.84	55.47	18.73
243	HOH	OH2	-41.21	-19.79	71.20	12.36
244	HOH	OH2	-47.90	-19.78	72.76	27.97
245	HOH	OH2	-42.20	-14.92	70.78	34.65
246	HOH	OH2	-26.14	-8.98	67.92	37.03
247	HOH	OH2	-32.81	-7.84	63.95	35.20
248	HOH	OH2	-19.95	-7.54	63.08	32.69
249	HOH	OH2	-16.19	-10.67	61.92	30.22
250	HOH	OH2	-35.01	-39.74	65.90	10.75
251	HOH	OH2	-13.63	-24.17	76.67	16.76
252	HOH	OH2	-8.21	-25.68	60.56	19.27
253	HOH	OH2	-20.14	-27.62	51.69	32.97
254	HOH	OH2	-25.01	-33.27	60.23	25.95
255	HOH	OH2	-13.56	-29.77	72.49	36.07
256	HOH	OH2	-33.43	-40.03	63.75	25.23
257	HOH	OH2	-20.84	-23.81	87.06	28.06
258	HOH	OH2	-13.50	-12.46	62.97	41.75
259	HOH	OH2	-28.41	-30.03	56.55	11.99
260	HOH	OH2	-28.87	-16.56	42.17	23.76
261	HOH	OH2	-25.56	-19.23	42.44	8.60
262	HOH	OH2	-32.08	-33.98	47.05	47.25
263	HOH	OH2	-22.35	-31.23	43.22	18.34
264	HOH	OH2	-32.62	-28.89	42.32	42.83
265	HOH	OH2	-38.09	-30.05	50.12	38.26

TABLE VIII

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for the cathepsin K complex with inhibitor 4-[N-[(4-pyridylmethoxy)carbonyl]-L-leucyl]-1-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-3-pyrrolidinone.

Residue Atom	X	Y	Z	B
1 ALA CB	-46.30	-38.07	64.13	15.00
1 ALA C	-48.64	-37.16	64.46	15.00
1 ALA O	-49.53	-37.68	63.79	15.00
1 ALA N	-48.10	-39.41	65.31	15.00
1 ALA CA	-47.55	-38.03	65.08	15.00
2 PRO N	-48.69	-35.88	64.81	15.00
2 PRO CD	-48.06	-35.33	66.02	15.00
2 PRO CA	-49.67	-34.93	64.29	15.00
2 PRO CB	-49.53	-33.73	65.24	15.00
2 PRO CG	-48.13	-33.85	65.77	15.00
2 PRO C	-49.42	-34.53	62.86	15.00
2 PRO O	-48.34	-34.77	62.28	15.00
3 ASP N	-50.40	-33.85	62.30	15.00
3 ASP CA	-50.29	-33.37	60.93	15.00
3 ASP CB	-51.65	-33.42	60.27	15.00
3 ASP CG	-52.12	-34.84	60.00	15.00
3 ASP OD1	-52.02	-35.30	58.84	15.00
3 ASP OD2	-52.59	-35.51	60.95	15.00
3 ASP C	-49.76	-31.93	61.01	15.00
3 ASP O	-49.44	-31.32	59.99	15.00
4 SER N	-49.58	-31.45	62.24	15.00
4 SER CA	-49.13	-30.09	62.51	15.00
4 SER CB	-50.32	-29.14	62.52	15.00
4 SER OG	-50.86	-29.02	61.20	15.00
4 SER C	-48.39	-29.96	63.84	15.00
4 SER O	-48.74	-30.63	64.84	15.00
5 VAL N	-47.34	-29.15	63.84	15.00
5 VAL CA	-46.50	-28.91	64.99	15.00
5 VAL CB	-45.35	-29.97	65.11	15.00
5 VAL CG1	-44.17	-29.43	65.89	15.00
5 VAL CG2	-45.84	-31.21	65.74	15.00
5 VAL C	-45.86	-27.57	64.80	15.00
5 VAL O	-45.37	-27.25	63.70	15.00

TABLE VIII

6 ASP N	-45.84	-26.80	65.89	15.00
6 ASP CA	-45.22	-25.50	65.92	15.00
6 ASP CB	-46.16	-24.37	65.46	15.00
6 ASP CG	-45.40	-23.07	65.15	15.00
6 ASP OD1	-44.21	-22.96	65.51	15.00
6 ASP OD2	-45.98	-22.17	64.51	15.00
6 ASP C	-44.81	-25.27	67.34	15.00
6 ASP O	-45.65	-24.96	68.17	15.00
7 TYR N	-43.51	-25.35	67.61	15.00
7 TYR CA	-43.00	-25.14	68.94	15.00
7 TYR CB	-41.63	-25.80	69.13	15.00
7 TYR CG	-41.68	-27.30	69.31	15.00
7 TYR CD1	-41.55	-27.88	70.57	15.00
7 TYR CE1	-41.60	-29.29	70.74	15.00
7 TYR CD2	-41.86	-28.14	68.22	15.00
7 TYR CE2	-41.91	-29.55	68.38	15.00
7 TYR CZ	-41.79	-30.10	69.64	15.00
7 TYR OH	-41.91	-31.46	69.83	15.00
7 TYR C	-42.85	-23.70	69.30	15.00
7 TYR O	-42.16	-23.39	70.26	15.00
8 ARG N	-43.40	-22.80	68.50	15.00
8 ARG CA	-43.31	-21.39	68.80	15.00
8 ARG CB	-43.55	-20.55	67.56	15.00
8 ARG CG	-42.37	-20.55	66.60	15.00
8 ARG CD	-42.57	-19.68	65.38	15.00
8 ARG NE	-43.64	-20.20	64.53	15.00
8 ARG CZ	-43.88	-19.78	63.29	15.00
8 ARG NH1	-43.09	-18.84	62.77	15.00
8 ARG NH2	-44.92	-20.26	62.60	15.00
8 ARG C	-44.37	-21.14	69.84	15.00
8 ARG O	-44.09	-20.64	70.93	15.00
9 LYS N	-45.58	-21.65	69.54	15.00
9 LYS CA	-46.73	-21.55	70.42	15.00
9 LYS CB	-47.95	-22.19	69.75	15.00
9 LYS CG	-48.42	-21.37	68.55	15.00
9 LYS CD	-48.71	-22.24	67.29	15.00
9 LYS CE	-49.41	-21.46	66.17	15.00
9 LYS NZ	-50.87	-21.36	66.45	15.00
9 LYS C	-46.44	-22.17	71.79	15.00
9 LYS O	-46.36	-21.45	72.77	15.00
10 LYS N	-46.15	-23.46	71.83	15.00
10 LYS CA	-45.85	-24.13	73.10	15.00
10 LYS CB	-45.43	-25.57	72.86	15.00

TABLE VIII

10	LYS	CG	-46.52	-26.39	72.25	15.00
10	LYS	CD	-46.05	-27.76	71.89	15.00
10	LYS	CE	-46.89	-28.35	70.81	15.00
10	LYS	NZ	-48.31	-27.94	70.92	15.00
10	LYS	C	-44.81	-23.41	73.94	15.00
10	LYS	O	-44.74	-23.62	75.14	15.00
11	GLY	N	-43.95	-22.63	73.30	15.00
11	GLY	CA	-42.94	-21.90	74.05	15.00
11	GLY	C	-41.53	-22.43	74.01	15.00
11	GLY	O	-40.78	-22.24	74.97	15.00
12	TYR	N	-41.13	-23.07	72.91	15.00
12	TYR	CA	-39.76	-23.60	72.84	15.00
12	TYR	CB	-39.78	-24.98	72.15	15.00
12	TYR	CG	-40.42	-26.09	72.97	15.00
12	TYR	CD1	-41.76	-26.06	73.35	15.00
12	TYR	CE1	-42.34	-27.10	74.13	15.00
12	TYR	CD2	-39.66	-27.18	73.39	15.00
12	TYR	CE2	-40.21	-28.21	74.17	15.00
12	TYR	CZ	-41.55	-28.17	74.53	15.00
12	TYR	OH	-42.10	-29.21	75.25	15.00
12	TYR	C	-38.82	-22.68	72.08	15.00
12	TYR	O	-37.64	-22.97	71.90	15.00
13	VAL	N	-39.37	-21.59	71.56	15.00
13	VAL	CA	-38.56	-20.71	70.75	15.00
13	VAL	CB	-39.14	-20.70	69.33	15.00
13	VAL	CG1	-38.15	-20.04	68.35	15.00
13	VAL	CG2	-39.49	-22.09	68.92	15.00
13	VAL	C	-38.31	-19.27	71.23	15.00
13	VAL	O	-39.24	-18.52	71.45	15.00
14	THR	N	-37.03	-18.90	71.32	15.00
14	THR	CA	-36.64	-17.56	71.76	15.00
14	THR	CB	-35.17	-17.57	72.25	15.00
14	THR	OG1	-34.33	-18.03	71.18	15.00
14	THR	CG2	-35.01	-18.43	73.50	15.00
14	THR	C	-36.70	-16.58	70.60	15.00
14	THR	O	-37.20	-16.92	69.53	15.00
15	PRO	N	-36.27	-15.32	70.83	15.00
15	PRO	CD	-36.21	-14.64	72.14	15.00
15	PRO	CA	-36.29	-14.32	69.76	15.00
15	PRO	CB	-35.98	-13.04	70.49	15.00
15	PRO	CG	-36.64	-13.24	71.83	15.00
15	PRO	C	-35.23	-14.60	68.72	15.00
15	PRO	O	-34.20	-15.21	69.02	15.00

TABLE VIII

16 VAL N	-35.48	-14.05	67.52	15.00
16 VAL CA	-34.61	-14.19	66.36	15.00
16 VAL CB	-35.37	-13.74	65.10	15.00
16 VAL CG1	-34.43	-13.61	63.92	15.00
16 VAL CG2	-36.44	-14.72	64.78	15.00
16 VAL C	-33.40	-13.33	66.56	15.00
16 VAL O	-33.47	-12.33	67.23	15.00
17 LYS N	-32.24	-13.78	66.10	15.00
17 LYS CA	-31.04	-12.97	66.26	15.00
17 LYS CB	-29.96	-13.71	67.06	15.00
17 LYS CG	-30.45	-14.44	68.35	15.00
17 LYS CD	-30.63	-13.52	69.54	15.00
17 LYS CE	-30.89	-14.30	70.82	15.00
17 LYS NZ	-32.14	-15.10	70.83	15.00
17 LYS C	-30.46	-12.58	64.91	15.00
17 LYS O	-31.06	-12.84	63.87	15.00
18 ASN N	-29.30	-11.94	64.94	15.00
18 ASN CA	-28.58	-11.48	63.75	15.00
18 ASN CB	-28.58	-9.96	63.69	15.00
18 ASN CG	-29.93	-9.39	63.96	15.00
18 ASN OD1	-30.89	-9.75	63.32	15.00
18 ASN ND2	-30.02	-8.56	64.97	15.00
18 ASN C	-27.16	-11.93	63.99	15.00
18 ASN O	-26.58	-11.59	65.03	15.00
19 GLN N	-26.59	-12.69	63.06	15.00
19 GLN CA	-25.22	-13.13	63.22	15.00
19 GLN CB	-24.96	-14.41	62.43	15.00
19 GLN CG	-25.34	-14.25	60.98	15.00
19 GLN CD	-25.10	-15.49	60.16	15.00
19 GLN OE1	-26.04	-16.20	59.82	15.00
19 GLN NE2	-23.86	-15.72	59.77	15.00
19 GLN C	-24.24	-12.02	62.83	15.00
19 GLN O	-23.05	-12.15	63.08	15.00
20 GLY N	-24.72	-11.01	62.11	15.00
20 GLY CA	-23.86	-9.91	61.69	15.00
20 GLY C	-22.83	-10.31	60.65	15.00
20 GLY O	-23.08	-11.26	59.94	15.00
21 GLN N	-21.69	-9.61	60.49	15.00
21 GLN CA	-20.72	-10.02	59.43	15.00
21 GLN CB	-20.01	-8.83	58.75	15.00
21 GLN CG	-20.87	-8.13	57.66	15.00
21 GLN CD	-21.58	-9.06	56.63	15.00
21 GLN OE1	-20.99	-10.02	56.16	15.00

TABLE VIII

21 GLN NE2	-22.84	-8.74	56.29	15.00
21 GLN C	-19.72	-11.10	59.87	15.00
21 GLN O	-18.50	-11.01	59.66	15.00
22 CYS N	-20.32	-12.22	60.26	15.00
22 CYS CA	-19.59	-13.37	60.72	15.00
22 CYS C	-20.26	-14.68	60.30	15.00
22 CYS O	-21.48	-14.80	60.28	15.00
22 CYS CB	-19.48	-13.22	62.25	15.00
22 CYS SG	-19.02	-14.67	63.24	15.00
23 GLY N	-19.45	-15.65	59.90	15.00
23 GLY CA	-20.01	-16.93	59.52	15.00
23 GLY C	-20.27	-17.81	60.75	15.00
23 GLY O	-19.73	-18.91	60.83	15.00
24 SER N	-21.20	-17.40	61.61	15.00
24 SER CA	-21.49	-18.12	62.84	15.00
24 SER CB	-21.32	-17.21	64.08	15.00
24 SER OG	-22.22	-16.10	64.07	15.00
24 SER C	-22.89	-18.73	62.86	15.00
24 SER O	-23.44	-19.03	63.90	15.00
25 CYS N	-23.46	-18.96	61.69	15.00
25 CYS CA	-24.78	-19.55	61.56	15.00
25 CYS CB	-25.18	-19.59	60.07	15.00
25 CYS SG	-24.19	-20.73	59.02	15.00
25 CYS C	-24.80	-20.92	62.24	15.00
25 CYS O	-25.77	-21.25	62.88	15.00
25 INH C1	-14.75	-27.52	59.81	15.00
25 INH C2	-15.58	-26.77	58.94	15.00
25 INH C3	-15.24	-25.44	58.65	15.00
25 INH C4	-14.06	-24.88	59.25	15.00
25 INH C5	-13.21	-25.64	60.14	15.00
25 INH C6	-13.57	-26.96	60.42	15.00
25 INH C7	-16.11	-24.63	57.72	15.00
25 INH O8	-17.39	-25.29	57.48	15.00
25 INH C9	-18.43	-24.53	57.00	15.00
25 INH O10	-18.33	-23.63	56.17	15.00
25 INH N11	-19.57	-24.86	57.54	15.00
25 INH C12	-20.88	-24.22	57.23	15.00
25 INH C13	-21.31	-23.29	58.42	15.00
25 INH N14	-21.06	-21.86	58.16	15.00
25 INH C15	-21.68	-21.41	56.87	15.00
25 INH C16	-21.59	-21.00	59.27	15.00
25 INH C17	-22.57	-20.07	58.55	15.00
25 INH C18	-22.15	-19.99	57.10	15.00

TABLE VIII

25	INH	C19	-21.87	-25.40	57.01	15.00
25	INH	C20	-22.73	-25.74	58.21	15.00
25	INH	C21	-22.94	-27.22	58.28	15.00
25	INH	C22	-24.00	-25.01	57.98	15.00
25	INH	N23	-23.18	-19.45	56.18	15.00
25	INH	C24	-23.12	-18.15	55.84	15.00
25	INH	O25	-22.20	-17.42	56.28	15.00
25	INH	C26	-24.25	-17.59	54.91	15.00
25	INH	C27	-24.00	-18.05	53.43	15.00
25	INH	C28	-25.22	-18.05	52.51	15.00
25	INH	C29	-25.14	-19.24	51.66	15.00
25	INH	C30	-25.25	-16.77	51.69	15.00
25	INH	N31	-24.30	-16.10	54.92	15.00
25	INH	C32	-24.85	-15.34	55.87	15.00
25	INH	O33	-25.40	-15.84	56.83	15.00
25	INH	O34	-24.72	-13.96	55.64	15.00
25	INH	C35	-24.74	-13.12	56.80	15.00
25	INH	C36	-25.68	-11.91	56.62	15.00
25	INH	C37	-25.21	-10.60	56.86	15.00
25	INH	C38	-26.09	-9.52	56.74	15.00
25	INH	N39	-27.37	-9.73	56.40	15.00
25	INH	C40	-27.85	-10.96	56.16	15.00
25	INH	C41	-27.03	-12.08	56.26	15.00
25	INH	O42	-22.66	-18.72	58.88	15.00
26	TRP	N	-23.72	-21.69	62.15	15.00
26	TRP	CA	-23.64	-23.01	62.85	15.00
26	TRP	CB	-22.30	-23.65	62.59	15.00
26	TRP	CG	-21.18	-22.75	63.06	15.00
26	TRP	CD2	-20.40	-22.85	64.28	15.00
26	TRP	CE2	-19.44	-21.79	64.22	15.00
26	TRP	CE3	-20.41	-23.71	65.38	15.00
26	TRP	CD1	-20.71	-21.70	62.39	15.00
26	TRP	NE1	-19.66	-21.12	63.05	15.00
26	TRP	CZ2	-18.49	-21.56	65.24	15.00
26	TRP	CZ3	-19.48	-23.49	66.41	15.00
26	TRP	CH2	-18.52	-22.41	66.33	15.00
26	TRP	C	-23.72	-22.83	64.40	15.00
26	TRP	O	-23.97	-23.79	65.16	15.00
27	ALA	N	-23.39	-21.64	64.91	15.00
27	ALA	CA	-23.50	-21.43	66.36	15.00
27	ALA	CB	-22.70	-20.24	66.80	15.00
27	ALA	C	-24.98	-21.21	66.72	15.00
27	ALA	O	-25.52	-21.89	67.60	15.00

TABLE VIII

28 PHE N	-25.63	-20.27	66.03	15.00
28 PHE CA	-27.02	-19.90	66.31	15.00
28 PHE CB	-27.46	-18.71	65.44	15.00
28 PHE CG	-26.88	-17.40	65.85	15.00
28 PHE CD1	-25.73	-16.87	65.27	15.00
28 PHE CD2	-27.47	-16.73	66.88	15.00
28 PHE CE1	-25.16	-15.71	65.70	15.00
28 PHE CE2	-26.92	-15.57	67.33	15.00
28 PHE CZ	-25.75	-15.04	66.75	15.00
28 PHE C	-27.93	-21.09	66.06	15.00
28 PHE O	-29.08	-21.05	66.44	15.00
29 SER N	-27.44	-22.09	65.33	15.00
29 SER CA	-28.24	-23.28	65.05	15.00
29 SER CB	-27.74	-23.99	63.81	15.00
29 SER OG	-28.44	-25.21	63.58	15.00
29 SER C	-28.13	-24.15	66.27	15.00
29 SER O	-29.14	-24.63	66.79	15.00
30 SER N	-26.90	-24.31	66.76	15.00
30 SER CA	-26.64	-25.13	67.94	15.00
30 SER CB	-25.14	-25.24	68.21	15.00
30 SER OG	-24.40	-25.67	67.06	15.00
30 SER C	-27.29	-24.63	69.21	15.00
30 SER O	-27.66	-25.40	70.08	15.00
31 VAL N	-27.31	-23.32	69.35	15.00
31 VAL CA	-27.89	-22.67	70.51	15.00
31 VAL CB	-27.39	-21.19	70.58	15.00
31 VAL CG1	-28.13	-20.34	71.59	15.00
31 VAL CG2	-25.91	-21.19	70.86	15.00
31 VAL C	-29.41	-22.80	70.55	15.00
31 VAL O	-30.02	-22.96	71.63	15.00
32 GLY N	-29.99	-22.81	69.35	15.00
32 GLY CA	-31.43	-22.91	69.21	15.00
32 GLY C	-31.90	-24.26	69.66	15.00
32 GLY O	-32.81	-24.39	70.47	15.00
33 ALA N	-31.22	-25.29	69.17	15.00
33 ALA CA	-31.51	-26.66	69.53	15.00
33 ALA CB	-30.58	-27.55	68.80	15.00
33 ALA C	-31.38	-26.86	71.06	15.00
33 ALA O	-32.23	-27.54	71.68	15.00
34 LEU N	-30.29	-26.34	71.63	15.00
34 LEU CA	-30.03	-26.45	73.05	15.00
34 LEU CB	-28.72	-25.82	73.41	15.00
34 LEU CG	-27.43	-26.58	73.17	15.00

TABLE VIII

34 LEU CD1	-26.28	-25.63	73.53	15.00
34 LEU CD2	-27.38	-27.85	74.05	15.00
34 LEU C	-31.12	-25.73	73.83	15.00
34 LEU O	-31.65	-26.29	74.80	15.00
35 GLU N	-31.47	-24.51	73.44	15.00
35 GLU CA	-32.54	-23.76	74.12	15.00
35 GLU CB	-32.78	-22.42	73.41	15.00
35 GLU CG	-31.67	-21.39	73.64	15.00
35 GLU CD	-31.63	-20.29	72.57	15.00
35 GLU OE1	-32.41	-20.37	71.57	15.00
35 GLU OE2	-30.81	-19.35	72.71	15.00
35 GLU C	-33.83	-24.57	74.20	15.00
35 GLU O	-34.34	-24.83	75.31	15.00
36 GLY N	-34.26	-25.10	73.05	15.00
36 GLY CA	-35.48	-25.91	72.99	15.00
36 GLY C	-35.58	-27.11	73.93	15.00
36 GLY O	-36.67	-27.47	74.37	15.00
37 GLN N	-34.44	-27.72	74.24	15.00
37 GLN CA	-34.40	-28.87	75.12	15.00
37 GLN CB	-33.06	-29.60	74.95	15.00
37 GLN CG	-32.79	-30.19	73.58	15.00
37 GLN CD	-33.83	-31.19	73.19	15.00
37 GLN OE1	-33.99	-32.23	73.84	15.00
37 GLN NE2	-34.56	-30.89	72.11	15.00
37 GLN C	-34.52	-28.38	76.55	15.00
37 GLN O	-35.01	-29.10	77.43	15.00
38 LEU N	-33.98	-27.18	76.79	15.00
38 LEU CA	-34.03	-26.60	78.12	15.00
38 LEU CB	-33.30	-25.26	78.14	15.00
38 LEU CG	-33.24	-24.54	79.47	15.00
38 LEU CD1	-32.61	-25.51	80.46	15.00
38 LEU CD2	-32.41	-23.30	79.36	15.00
38 LEU C	-35.46	-26.45	78.60	15.00
38 LEU O	-35.86	-27.10	79.58	15.00
39 LYS N	-36.26	-25.70	77.84	15.00
39 LYS CA	-37.68	-25.45	78.15	15.00
39 LYS CB	-38.34	-24.71	76.97	15.00
39 LYS CG	-39.49	-23.74	77.33	15.00
39 LYS CD	-40.74	-24.43	77.83	15.00
39 LYS CE	-41.85	-23.45	78.12	15.00
39 LYS NZ	-41.65	-22.78	79.42	15.00
39 LYS C	-38.42	-26.78	78.46	15.00
39 LYS O	-39.33	-26.82	79.30	15.00

TABLE VIII

40	LYS	N	-38.04	-27.84	77.77	15.00
40	LYS	CA	-38.66	-29.14	77.99	15.00
40	LYS	CB	-38.41	-30.07	76.81	15.00
40	LYS	CG	-39.57	-31.02	76.53	15.00
40	LYS	CD	-39.10	-32.29	75.82	15.00
40	LYS	CE	-40.02	-32.72	74.68	15.00
40	LYS	NZ	-40.21	-31.65	73.65	15.00
40	LYS	C	-38.08	-29.74	79.27	15.00
40	LYS	O	-38.79	-30.27	80.12	15.00
41	LYS	N	-36.77	-29.60	79.41	15.00
41	LYS	CA	-36.05	-30.13	80.55	15.00
41	LYS	CB	-34.53	-29.93	80.33	15.00
41	LYS	CG	-33.63	-30.86	81.11	15.00
41	LYS	CD	-33.79	-32.26	80.55	15.00
41	LYS	CE	-33.13	-33.31	81.42	15.00
41	LYS	NZ	-33.45	-34.68	80.86	15.00
41	LYS	C	-36.49	-29.45	81.84	15.00
41	LYS	O	-37.34	-29.97	82.61	15.00
42	THR	N	-35.96	-28.25	82.04	15.00
42	THR	CA	-36.22	-27.48	83.24	15.00
42	THR	CB	-34.87	-26.94	83.78	15.00
42	THR	OG1	-34.35	-25.91	82.92	15.00
42	THR	CG2	-33.86	-28.07	83.79	15.00
42	THR	C	-37.16	-26.30	83.02	15.00
42	THR	O	-36.86	-25.20	83.45	15.00
43	GLY	N	-38.28	-26.52	82.34	15.00
43	GLY	CA	-39.26	-25.47	82.12	15.00
43	GLY	C	-38.87	-24.03	81.79	15.00
43	GLY	O	-39.77	-23.21	81.54	15.00
44	LYS	N	-37.56	-23.75	81.75	15.00
44	LYS	CA	-37.02	-22.41	81.49	15.00
44	LYS	CB	-35.84	-22.13	82.44	15.00
44	LYS	CG	-36.25	-21.41	83.72	15.00
44	LYS	CD	-35.09	-21.25	84.67	15.00
44	LYS	CE	-35.50	-20.36	85.86	15.00
44	LYS	NZ	-36.56	-20.99	86.66	15.00
44	LYS	C	-36.56	-22.13	80.06	15.00
44	LYS	O	-35.71	-22.83	79.51	15.00
45	LEU	N	-37.07	-21.04	79.50	15.00
45	LEU	CA	-36.70	-20.66	78.14	15.00
45	LEU	CB	-37.93	-20.08	77.46	15.00
45	LEU	CG	-38.06	-19.92	75.94	15.00
45	LEU	CD1	-37.93	-21.25	75.26	15.00

TABLE VIII

45	LEU	CD2	-39.40	-19.29	75.63	15.00
45	LEU	C	-35.66	-19.57	78.35	15.00
45	LEU	O	-36.00	-18.46	78.71	15.00
46	LEU	N	-34.40	-19.94	78.29	15.00
46	LEU	CA	-33.30	-18.99	78.50	15.00
46	LEU	CB	-32.23	-19.62	79.41	15.00
46	LEU	CG	-31.90	-18.84	80.70	15.00
46	LEU	CD1	-32.48	-19.56	81.88	15.00
46	LEU	CD2	-30.35	-18.72	80.89	15.00
46	LEU	C	-32.68	-18.70	77.13	15.00
46	LEU	O	-32.93	-19.45	76.19	15.00
47	ASN	N	-31.92	-17.61	76.99	15.00
47	ASN	CA	-31.23	-17.30	75.73	15.00
47	ASN	CB	-31.29	-15.79	75.44	15.00
47	ASN	CG	-32.61	-15.36	74.77	15.00
47	ASN	OD1	-32.68	-15.24	73.55	15.00
47	ASN	ND2	-33.63	-15.06	75.58	15.00
47	ASN	C	-29.74	-17.70	75.90	15.00
47	ASN	O	-29.01	-16.99	76.58	15.00
48	LEU	N	-29.28	-18.80	75.29	15.00
48	LEU	CA	-27.88	-19.20	75.45	15.00
48	LEU	CB	-27.67	-20.68	75.16	15.00
48	LEU	CG	-28.05	-21.69	76.27	15.00
48	LEU	CD1	-27.81	-21.07	77.65	15.00
48	LEU	CD2	-29.49	-22.12	76.12	15.00
48	LEU	C	-26.85	-18.34	74.73	15.00
48	LEU	O	-27.20	-17.31	74.23	15.00
49	SER	N	-25.58	-18.70	74.74	15.00
49	SER	CA	-24.59	-17.83	74.11	15.00
49	SER	CB	-23.51	-17.50	75.14	15.00
49	SER	OG	-22.32	-17.09	74.51	15.00
49	SER	C	-23.93	-18.37	72.87	15.00
49	SER	O	-23.08	-19.27	72.98	15.00
50	PRO	N	-24.29	-17.86	71.67	15.00
50	PRO	CD	-25.31	-16.83	71.34	15.00
50	PRO	CA	-23.66	-18.36	70.45	15.00
50	PRO	CB	-24.47	-17.67	69.35	15.00
50	PRO	CG	-24.96	-16.44	69.97	15.00
50	PRO	C	-22.18	-17.94	70.44	15.00
50	PRO	O	-21.36	-18.62	69.86	15.00
51	GLN	N	-21.82	-16.87	71.13	15.00
51	GLN	CA	-20.43	-16.41	71.17	15.00
51	GLN	CB	-20.39	-14.98	71.74	15.00

TABLE VIII

51 GLN CG	-19.02	-14.25	71.69	15.00
51 GLN CD	-18.76	-13.61	70.35	15.00
51 GLN OE1	-19.65	-12.97	69.76	15.00
51 GLN NE2	-17.54	-13.79	69.84	15.00
51 GLN C	-19.46	-17.34	71.94	15.00
51 GLN O	-18.31	-17.50	71.53	15.00
52 ASN N	-19.90	-17.99	73.02	15.00
52 ASN CA	-19.02	-18.91	73.78	15.00
52 ASN CB	-19.79	-19.58	74.91	15.00
52 ASN CG	-18.92	-20.56	75.72	15.00
52 ASN OD1	-19.45	-21.25	76.60	15.00
52 ASN ND2	-17.61	-20.58	75.49	15.00
52 ASN C	-18.54	-19.96	72.80	15.00
52 ASN O	-17.34	-20.22	72.69	15.00
53 LEU N	-19.50	-20.50	72.05	15.00
53 LEU CA	-19.28	-21.52	71.00	15.00
53 LEU CB	-20.62	-21.86	70.33	15.00
53 LEU CG	-21.43	-23.10	70.69	15.00
53 LEU CD1	-21.19	-23.59	72.12	15.00
53 LEU CD2	-22.91	-22.80	70.38	15.00
53 LEU C	-18.28	-21.04	69.94	15.00
53 LEU O	-17.34	-21.76	69.60	15.00
54 VAL N	-18.48	-19.82	69.46	15.00
54 VAL CA	-17.63	-19.27	68.44	15.00
54 VAL CB	-18.01	-17.82	68.09	15.00
54 VAL CG1	-16.94	-17.17	67.25	15.00
54 VAL CG2	-19.32	-17.76	67.40	15.00
54 VAL C	-16.18	-19.32	68.84	15.00
54 VAL O	-15.36	-19.90	68.11	15.00
55 ASP N	-15.88	-18.75	70.02	15.00
55 ASP CA	-14.53	-18.65	70.58	15.00
55 ASP CB	-14.49	-17.73	71.81	15.00
55 ASP CG	-14.86	-16.30	71.52	15.00
55 ASP OD1	-14.87	-15.89	70.35	15.00
55 ASP OD2	-15.13	-15.56	72.49	15.00
55 ASP C	-13.87	-19.93	71.08	15.00
55 ASP O	-12.65	-20.14	70.82	15.00
56 CYS N	-14.62	-20.75	71.81	15.00
56 CYS CA	-14.06	-21.94	72.42	15.00
56 CYS C	-14.14	-23.23	71.62	15.00
56 CYS O	-13.36	-24.15	71.85	15.00
56 CYS CB	-14.74	-22.17	73.76	15.00
56 CYS SG	-14.67	-20.81	74.99	15.00

TABLE VIII

57 VAL N	-15.00	-23.30	70.62	15.00
57 VAL CA	-15.09	-24.53	69.88	15.00
57 VAL CB	-16.51	-24.71	69.30	15.00
57 VAL CG1	-16.66	-26.03	68.70	15.00
57 VAL CG2	-17.56	-24.53	70.42	15.00
57 VAL C	-13.92	-24.66	68.88	15.00
57 VAL O	-14.05	-24.47	67.68	15.00
58 SER N	-12.79	-25.08	69.43	15.00
58 SER CA	-11.51	-25.26	68.71	15.00
58 SER CB	-10.43	-25.78	69.66	15.00
58 SER OG	-9.18	-25.96	68.99	15.00
58 SER C	-11.53	-26.13	67.45	15.00
58 SER O	-10.66	-26.01	66.58	15.00
59 GLU N	-12.54	-26.98	67.36	15.00
59 GLU CA	-12.67	-27.86	66.21	15.00
59 GLU CB	-13.47	-29.12	66.60	15.00
59 GLU CG	-13.12	-29.70	68.00	15.00
59 GLU CD	-14.02	-29.15	69.13	15.00
59 GLU OE1	-15.16	-29.68	69.29	15.00
59 GLU OE2	-13.56	-28.20	69.84	15.00
59 GLU C	-13.30	-27.07	65.05	15.00
59 GLU O	-13.21	-27.46	63.91	15.00
60 ASN N	-13.91	-25.93	65.35	15.00
60 ASN CA	-14.50	-25.14	64.28	15.00
60 ASN CB	-15.92	-24.71	64.63	15.00
60 ASN CG	-16.96	-25.87	64.48	15.00
60 ASN OD1	-17.94	-25.95	65.23	15.00
60 ASN ND2	-16.75	-26.74	63.50	15.00
60 ASN C	-13.60	-23.94	63.89	15.00
60 ASN O	-12.43	-23.91	64.25	15.00
61 ASP N	-14.11	-23.06	63.02	15.00
61 ASP CA	-13.36	-21.90	62.53	15.00
61 ASP CB	-13.29	-21.96	61.02	15.00
61 ASP CG	-11.96	-22.46	60.52	15.00
61 ASP OD1	-11.41	-23.42	61.13	15.00
61 ASP OD2	-11.48	-21.91	59.50	15.00
61 ASP C	-13.89	-20.55	62.98	15.00
61 ASP O	-13.38	-19.49	62.62	15.00
62 GLY N	-14.94	-20.59	63.77	15.00
62 GLY CA	-15.48	-19.35	64.30	15.00
62 GLY C	-16.16	-18.55	63.21	15.00
62 GLY O	-17.14	-19.03	62.59	15.00
63 CYS N	-15.70	-17.33	62.93	15.00

TABLE VIII

63 CYS CA	-16.40	-16.58	61.91	15.00
63 CYS C	-16.18	-17.07	60.50	15.00
63 CYS O	-16.75	-16.57	59.55	15.00
63 CYS CB	-16.13	-15.11	62.08	15.00
63 CYS SG	-17.00	-14.35	63.54	15.00
64 GLY N	-15.46	-18.19	60.41	15.00
64 GLY CA	-15.19	-18.79	59.11	15.00
64 GLY C	-16.12	-19.97	58.83	15.00
64 GLY O	-16.19	-20.49	57.72	15.00
65 GLY N	-16.79	-20.46	59.86	15.00
65 GLY CA	-17.70	-21.56	59.62	15.00
65 GLY C	-17.39	-22.81	60.42	15.00
65 GLY O	-16.24	-23.13	60.74	15.00
66 GLY N	-18.43	-23.62	60.61	15.00
66 GLY CA	-18.29	-24.85	61.37	15.00
66 GLY C	-19.48	-25.78	61.43	15.00
66 GLY O	-20.57	-25.37	61.00	15.00
67 TYR N	-19.31	-26.94	62.06	15.00
67 TYR CA	-20.37	-27.91	62.16	15.00
67 TYR CB	-19.83	-29.31	61.82	15.00
67 TYR CG	-19.28	-29.38	60.43	15.00
67 TYR CD1	-20.08	-29.14	59.33	15.00
67 TYR CE1	-19.54	-29.09	58.03	15.00
67 TYR CD2	-17.93	-29.57	60.21	15.00
67 TYR CE2	-17.39	-29.52	58.91	15.00
67 TYR CZ	-18.20	-29.27	57.84	15.00
67 TYR OH	-17.70	-29.21	56.59	15.00
67 TYR C	-21.11	-27.86	63.49	15.00
67 TYR O	-20.55	-27.52	64.52	15.00
68 MET N	-22.40	-28.13	63.48	15.00
68 MET CA	-23.12	-28.14	64.76	15.00
68 MET CB	-24.62	-28.23	64.56	15.00
68 MET CG	-25.11	-27.02	63.82	15.00
68 MET SD	-24.76	-27.31	62.04	15.00
68 MET CE	-26.39	-28.14	61.56	15.00
68 MET C	-22.66	-29.31	65.63	15.00
68 MET O	-22.63	-29.21	66.83	15.00
69 THR N	-22.32	-30.42	64.99	15.00
69 THR CA	-21.87	-31.57	65.74	15.00
69 THR CB	-21.55	-32.78	64.81	15.00
69 THR OG1	-20.68	-32.38	63.72	15.00
69 THR CG2	-22.82	-33.41	64.29	15.00
69 THR C	-20.65	-31.21	66.61	15.00

TABLE VIII

69 THR O	-20.61	-31.62	67.76	15.00
70 ASN N	-19.74	-30.38	66.11	15.00
70 ASN CA	-18.56	-30.05	66.91	15.00
70 ASN CB	-17.53	-29.28	66.07	15.00
70 ASN CG	-16.83	-30.17	65.02	15.00
70 ASN OD1	-17.07	-31.39	64.94	15.00
70 ASN ND2	-16.02	-29.55	64.17	15.00
70 ASN C	-18.99	-29.22	68.11	15.00
70 ASN O	-18.59	-29.49	69.21	15.00
71 ALA N	-19.95	-28.33	67.87	15.00
71 ALA CA	-20.42	-27.44	68.91	15.00
71 ALA CB	-21.27	-26.35	68.33	15.00
71 ALA C	-21.15	-28.13	70.05	15.00
71 ALA O	-21.13	-27.69	71.20	15.00
72 PHE N	-21.84	-29.22	69.71	15.00
72 PHE CA	-22.53	-29.99	70.74	15.00
72 PHE CB	-23.59	-30.93	70.13	15.00
72 PHE CG	-24.75	-30.22	69.47	15.00
72 PHE CD1	-25.59	-29.41	70.21	15.00
72 PHE CD2	-25.05	-30.41	68.12	15.00
72 PHE CE1	-26.70	-28.82	69.63	15.00
72 PHE CE2	-26.16	-29.82	67.55	15.00
72 PHE CZ	-26.97	-29.03	68.31	15.00
72 PHE C	-21.49	-30.80	71.51	15.00
72 PHE O	-21.54	-30.91	72.73	15.00
73 GLN N	-20.55	-31.39	70.78	15.00
73 GLN CA	-19.50	-32.16	71.39	15.00
73 GLN CB	-18.48	-32.63	70.34	15.00
73 GLN CG	-17.59	-33.74	70.84	15.00
73 GLN CD	-17.19	-34.69	69.73	15.00
73 GLN OE1	-17.48	-35.89	69.78	15.00
73 GLN NE2	-16.52	-34.16	68.72	15.00
73 GLN C	-18.81	-31.26	72.43	15.00
73 GLN O	-18.64	-31.64	73.59	15.00
74 TYR N	-18.39	-30.06	72.02	15.00
74 TYR CA	-17.70	-29.17	72.97	15.00
74 TYR CB	-17.27	-27.85	72.29	15.00
74 TYR CG	-17.25	-26.64	73.21	15.00
74 TYR CD1	-16.09	-26.24	73.83	15.00
74 TYR CE1	-16.11	-25.21	74.74	15.00
74 TYR CD2	-18.43	-25.98	73.51	15.00
74 TYR CE2	-18.46	-24.94	74.43	15.00
74 TYR CZ	-17.30	-24.57	75.05	15.00

TABLE VIII

74 TYR OH	-17.27	-23.57	76.01	15.00
74 TYR C	-18.51	-28.95	74.27	15.00
74 TYR O	-18.01	-29.19	75.35	15.00
75 VAL N	-19.77	-28.61	74.13	15.00
75 VAL CA	-20.68	-28.40	75.27	15.00
75 VAL CB	-22.10	-28.09	74.67	15.00
75 VAL CG1	-23.21	-28.24	75.71	15.00
75 VAL CG2	-22.09	-26.67	74.09	15.00
75 VAL C	-20.70	-29.59	76.29	15.00
75 VAL O	-21.29	-29.50	77.38	15.00
76 GLN N	-20.09	-30.71	75.88	15.00
76 GLN CA	-20.03	-31.93	76.68	15.00
76 GLN CB	-20.30	-33.15	75.77	15.00
76 GLN CG	-20.03	-34.52	76.35	15.00
76 GLN CD	-20.70	-35.58	75.54	15.00
76 GLN OE1	-21.76	-36.09	75.93	15.00
76 GLN NE2	-20.15	-35.88	74.37	15.00
76 GLN C	-18.70	-32.10	77.39	15.00
76 GLN O	-18.66	-32.13	78.61	15.00
77 LYS N	-17.61	-32.20	76.65	15.00
77 LYS CA	-16.31	-32.37	77.28	15.00
77 LYS CB	-15.24	-32.65	76.24	15.00
77 LYS CG	-15.60	-33.84	75.35	15.00
77 LYS CD	-14.38	-34.57	74.81	15.00
77 LYS CE	-13.52	-33.71	73.91	15.00
77 LYS NZ	-12.57	-34.54	73.09	15.00
77 LYS C	-15.94	-31.16	78.15	15.00
77 LYS O	-15.31	-31.32	79.19	15.00
78 ASN N	-16.35	-29.96	77.75	15.00
78 ASN CA	-16.09	-28.77	78.57	15.00
78 ASN CB	-16.09	-27.49	77.72	15.00
78 ASN CG	-16.13	-26.22	78.58	15.00
78 ASN OD1	-15.14	-25.84	79.17	15.00
78 ASN ND2	-17.32	-25.64	78.72	15.00
78 ASN C	-17.17	-28.68	79.66	15.00
78 ASN O	-17.18	-27.77	80.49	15.00
79 ARG N	-18.08	-29.64	79.64	15.00
79 ARG CA	-19.18	-29.69	80.60	15.00
79 ARG CB	-18.69	-30.15	81.98	15.00
79 ARG CG	-18.36	-31.63	82.12	15.00
79 ARG CD	-17.79	-31.93	83.52	15.00
79 ARG NE	-16.63	-32.84	83.47	15.00
79 ARG CZ	-15.39	-32.46	83.15	15.00

TABLE VIII

79 ARG NH1	-15.15	-31.19	82.86	15.00
79 ARG NH2	-14.38	-33.34	83.16	15.00
79 ARG C	-20.00	-28.40	80.78	15.00
79 ARG O	-20.27	-27.99	81.91	15.00
80 GLY N	-20.32	-27.70	79.70	15.00
80 GLY CA	-21.14	-26.50	79.88	15.00
80 GLY C	-21.02	-25.34	78.91	15.00
80 GLY O	-19.94	-25.13	78.31	15.00
81 ILE N	-22.13	-24.60	78.78	15.00
81 ILE CA	-22.27	-23.43	77.92	15.00
81 ILE CB	-23.18	-23.77	76.69	15.00
81 ILE CG2	-24.60	-24.14	77.13	15.00
81 ILE CG1	-23.28	-22.57	75.76	15.00
81 ILE CD1	-24.04	-22.84	74.48	15.00
81 ILE C	-22.91	-22.32	78.75	15.00
81 ILE O	-23.73	-22.62	79.63	15.00
82 ASP N	-22.58	-21.05	78.48	15.00
82 ASP CA	-23.13	-19.92	79.28	15.00
82 ASP CB	-22.13	-18.77	79.29	15.00
82 ASP CG	-20.88	-19.11	80.02	15.00
82 ASP OD1	-19.80	-18.87	79.48	15.00
82 ASP OD2	-20.96	-19.62	81.14	15.00
82 ASP C	-24.47	-19.36	78.83	15.00
82 ASP O	-25.10	-19.90	77.94	15.00
83 SER N	-24.92	-18.31	79.51	15.00
83 SER CA	-26.12	-17.57	79.18	15.00
83 SER CB	-26.70	-16.97	80.48	15.00
83 SER OG	-25.68	-16.38	81.28	15.00
83 SER C	-25.55	-16.45	78.27	15.00
83 SER O	-24.33	-16.24	78.28	15.00
84 GLU N	-26.35	-15.82	77.39	15.00
84 GLU CA	-25.85	-14.72	76.54	15.00
84 GLU CB	-27.00	-13.88	75.94	15.00
84 GLU CG	-27.12	-13.72	74.39	15.00
84 GLU CD	-25.97	-12.97	73.70	15.00
84 GLU OE1	-25.80	-11.74	73.90	15.00
84 GLU OE2	-25.23	-13.64	72.93	15.00
84 GLU C	-25.15	-13.79	77.53	15.00
84 GLU O	-24.00	-13.44	77.37	15.00
85 ASP N	-25.85	-13.43	78.61	15.00
85 ASP CA	-25.31	-12.53	79.65	15.00
85 ASP CB	-26.08	-12.68	80.98	15.00
85 ASP CG	-27.48	-12.06	80.94	15.00

TABLE VIII

85 ASP OD1	-28.41	-12.76	81.40	15.00
85 ASP OD2	-27.63	-10.90	80.45	15.00
85 ASP C	-23.80	-12.67	79.97	15.00
85 ASP O	-23.07	-11.67	80.00	15.00
86 ALA N	-23.36	-13.90	80.22	15.00
86 ALA CA	-21.96	-14.21	80.59	15.00
86 ALA CB	-21.89	-15.55	81.31	15.00
86 ALA C	-21.00	-14.20	79.40	15.00
86 ALA O	-19.76	-14.22	79.57	15.00
87 TYR N	-21.55	-14.11	78.20	15.00
87 TYR CA	-20.74	-14.13	76.99	15.00
87 TYR CB	-20.41	-15.60	76.66	15.00
87 TYR CG	-18.96	-15.90	76.36	15.00
87 TYR CD1	-18.23	-15.14	75.50	15.00
87 TYR CE1	-16.93	-15.44	75.21	15.00
87 TYR CD2	-18.34	-16.98	76.94	15.00
87 TYR CE2	-17.04	-17.27	76.65	15.00
87 TYR CZ	-16.35	-16.52	75.79	15.00
87 TYR OH	-15.09	-16.87	75.41	15.00
87 TYR C	-21.57	-13.50	75.86	15.00
87 TYR O	-21.88	-14.19	74.89	15.00
88 PRO N	-21.98	-12.22	75.98	15.00
88 PRO CD	-21.70	-11.28	77.08	15.00
88 PRO CA	-22.78	-11.57	74.93	15.00
88 PRO CB	-22.84	-10.11	75.41	15.00
88 PRO CG	-22.78	-10.21	76.93	15.00
88 PRO C	-22.14	-11.72	73.54	15.00
88 PRO O	-20.91	-11.95	73.44	15.00
89 TYR N	-22.97	-11.62	72.49	15.00
89 TYR CA	-22.50	-11.76	71.11	15.00
89 TYR CB	-23.64	-12.25	70.22	15.00
89 TYR CG	-23.22	-12.67	68.82	15.00
89 TYR CD1	-22.42	-13.82	68.64	15.00
89 TYR CE1	-22.03	-14.24	67.35	15.00
89 TYR CD2	-23.62	-11.92	67.68	15.00
89 TYR CE2	-23.24	-12.31	66.41	15.00
89 TYR CZ	-22.44	-13.47	66.24	15.00
89 TYR OH	-22.00	-13.78	64.96	15.00
89 TYR C	-21.91	-10.45	70.58	15.00
89 TYR O	-22.53	-9.40	70.70	15.00
90 VAL N	-20.67	-10.51	70.08	15.00
90 VAL CA	-19.98	-9.36	69.50	15.00
90 VAL CB	-18.74	-8.92	70.32	15.00

TABLE VIII

90 VAL CG1	-19.17	-8.55	71.75	15.00
90 VAL CG2	-17.66	-9.99	70.28	15.00
90 VAL C	-19.58	-9.60	68.03	15.00
90 VAL O	-18.77	-8.86	67.47	15.00
91 GLY N	-20.12	-10.65	67.43	15.00
91 GLY CA	-19.85	-10.97	66.03	15.00
91 GLY C	-18.40	-10.89	65.56	15.00
91 GLY O	-18.09	-10.75	64.36	15.00
92 GLN N	-17.49	-11.02	66.50	15.00
92 GLN CA	-16.08	-10.99	66.22	15.00
92 GLN CB	-15.44	-9.73	66.78	15.00
92 GLN CG	-14.07	-9.49	66.26	15.00
92 GLN CD	-13.74	-8.01	66.30	15.00
92 GLN OE1	-13.84	-7.29	65.30	15.00
92 GLN NE2	-13.35	-7.54	67.49	15.00
92 GLN C	-15.63	-12.18	67.00	15.00
92 GLN O	-16.16	-12.45	68.08	15.00
93 GLU N	-14.75	-12.96	66.42	15.00
93 GLU CA	-14.27	-14.11	67.13	15.00
93 GLU CB	-13.67	-15.14	66.19	15.00
93 GLU CG	-13.54	-16.51	66.82	15.00
93 GLU CD	-12.31	-17.23	66.33	15.00
93 GLU OE1	-11.79	-18.11	67.03	15.00
93 GLU OE2	-11.86	-16.90	65.23	15.00
93 GLU C	-13.17	-13.56	68.00	15.00
93 GLU O	-12.58	-12.52	67.67	15.00
94 GLU N	-12.98	-14.19	69.17	15.00
94 GLU CA	-11.95	-13.83	70.12	15.00
94 GLU CB	-12.45	-12.76	71.08	15.00
94 GLU CG	-13.44	-11.78	70.55	15.00
94 GLU CD	-13.36	-10.49	71.28	15.00
94 GLU OE1	-12.35	-9.77	71.16	15.00
94 GLU OE2	-14.28	-10.18	72.03	15.00
94 GLU C	-11.52	-15.03	70.95	15.00
94 GLU O	-12.21	-16.05	71.03	15.00
95 SER N	-10.46	-14.79	71.73	15.00
95 SER CA	-9.89	-15.79	72.60	15.00
95 SER CB	-8.61	-15.24	73.23	15.00
95 SER OG	-7.71	-14.80	72.23	15.00
95 SER C	-10.92	-16.24	73.63	15.00
95 SER O	-11.66	-15.42	74.18	15.00
96 CYS N	-10.99	-17.55	73.82	15.00
96 CYS CA	-11.94	-18.19	74.74	15.00

TABLE VIII

96 CYS C	-11.83	-17.70	76.17	15.00
96 CYS O	-10.75	-17.73	76.79	15.00
96 CYS CB	-11.80	-19.73	74.68	15.00
96 CYS SG	-12.78	-20.81	75.78	15.00
97 MET N	-12.97	-17.26	76.69	15.00
97 MET CA	-13.10	-16.73	78.03	15.00
97 MET CB	-13.17	-15.20	78.02	15.00
97 MET CG	-12.67	-14.49	79.27	15.00
97 MET SD	-10.82	-14.26	79.19	15.00
97 MET CE	-10.31	-15.40	80.50	15.00
97 MET C	-14.34	-17.32	78.74	15.00
97 MET O	-15.06	-16.60	79.42	15.00
98 TYR N	-14.60	-18.61	78.59	15.00
98 TYR CA	-15.74	-19.28	79.24	15.00
98 TYR CB	-15.63	-20.78	79.00	15.00
98 TYR CG	-16.63	-21.59	79.77	15.00
98 TYR CD1	-17.98	-21.47	79.50	15.00
98 TYR CE1	-18.91	-22.15	80.24	15.00
98 TYR CD2	-16.22	-22.44	80.82	15.00
98 TYR CE2	-17.15	-23.16	81.58	15.00
98 TYR CZ	-18.51	-22.99	81.27	15.00
98 TYR OH	-19.51	-23.63	81.97	15.00
98 TYR C	-15.85	-19.00	80.73	15.00
98 TYR O	-14.85	-18.70	81.38	15.00
99 ASN N	-17.06	-19.08	81.26	15.00
99 ASN CA	-17.25	-18.79	82.67	15.00
99 ASN CB	-17.77	-17.37	82.86	15.00
99 ASN CG	-17.78	-16.95	84.33	15.00
99 ASN OD1	-18.62	-17.40	85.11	15.00
99 ASN ND2	-16.82	-16.11	84.70	15.00
99 ASN C	-18.13	-19.73	83.47	15.00
99 ASN O	-19.36	-19.70	83.36	15.00
100 PRO N	-17.51	-20.60	84.28	15.00
100 PRO CD	-16.06	-20.90	84.34	15.00
100 PRO CA	-18.26	-21.55	85.10	15.00
100 PRO CB	-17.25	-21.89	86.20	15.00
100 PRO CG	-15.98	-22.00	85.45	15.00
100 PRO C	-19.56	-21.03	85.71	15.00
100 PRO O	-20.61	-21.68	85.55	15.00
101 THR N	-19.48	-19.89	86.41	15.00
101 THR CA	-20.63	-19.30	87.10	15.00
101 THR CB	-20.18	-18.20	88.13	15.00
101 THR OG1	-19.04	-17.45	87.66	15.00

TABLE VIII

101 THR CG2	-19.82	-18.87	89.46	15.00
101 THR C	-21.77	-18.86	86.17	15.00
101 THR O	-22.95	-18.78	86.56	15.00
102 GLY N	-21.40	-18.68	84.91	15.00
102 GLY CA	-22.35	-18.33	83.88	15.00
102 GLY C	-23.27	-19.50	83.58	15.00
102 GLY O	-24.47	-19.30	83.42	15.00
103 LYS N	-22.68	-20.69	83.38	15.00
103 LYS CA	-23.39	-21.95	83.13	15.00
103 LYS CB	-22.95	-23.01	84.16	15.00
103 LYS CG	-23.73	-24.31	84.12	15.00
103 LYS CD	-23.11	-25.38	85.05	15.00
103 LYS CE	-21.69	-25.76	84.61	15.00
103 LYS NZ	-21.01	-26.68	85.56	15.00
103 LYS C	-24.90	-21.82	83.20	15.00
103 LYS O	-25.45	-21.45	84.23	15.00
104 ALA N	-25.58	-22.16	82.10	15.00
104 ALA CA	-27.05	-22.11	82.04	15.00
104 ALA CB	-27.54	-20.84	81.26	15.00
104 ALA C	-27.64	-23.39	81.42	15.00
104 ALA O	-28.85	-23.61	81.42	15.00
105 ALA N	-26.79	-24.26	80.92	15.00
105 ALA CA	-27.24	-25.50	80.30	15.00
105 ALA CB	-28.05	-25.22	79.03	15.00
105 ALA C	-26.03	-26.35	79.97	15.00
105 ALA O	-24.88	-25.90	80.04	15.00
106 LYS N	-26.32	-27.59	79.60	15.00
106 LYS CA	-25.32	-28.57	79.25	15.00
106 LYS CB	-24.74	-29.13	80.55	15.00
106 LYS CG	-23.71	-30.22	80.42	15.00
106 LYS CD	-23.54	-30.96	81.75	15.00
106 LYS CE	-24.85	-31.60	82.15	15.00
106 LYS NZ	-24.61	-32.90	82.82	15.00
106 LYS C	-26.09	-29.63	78.43	15.00
106 LYS O	-27.32	-29.62	78.34	15.00
107 CYS N	-25.36	-30.51	77.77	15.00
107 CYS CA	-26.00	-31.54	76.97	15.00
107 CYS CB	-26.06	-31.11	75.50	15.00
107 CYS SG	-24.54	-31.49	74.55	15.00
107 CYS C	-25.07	-32.72	77.10	15.00
107 CYS O	-23.85	-32.54	77.25	15.00
108 ARG N	-25.62	-33.92	77.06	15.00
108 ARG CA	-24.80	-35.12	77.17	15.00

TABLE VIII

108 ARG CB	-25.28	-36.03	78.28	15.00
108 ARG CG	-25.35	-35.42	79.64	15.00
108 ARG CD	-25.75	-36.49	80.66	15.00
108 ARG NE	-27.18	-36.72	80.71	15.00
108 ARG CZ	-27.75	-37.86	81.09	15.00
108 ARG NH1	-27.00	-38.90	81.43	15.00
108 ARG NH2	-29.07	-37.94	81.22	15.00
108 ARG C	-24.85	-35.89	75.85	15.00
108 ARG O	-25.59	-36.87	75.72	15.00
109 GLY N	-24.11	-35.40	74.87	15.00
109 GLY CA	-24.05	-36.03	73.57	15.00
109 GLY C	-24.99	-35.44	72.55	15.00
109 GLY O	-25.58	-34.38	72.78	15.00
110 TYR N	-25.00	-36.06	71.36	15.00
110 TYR CA	-25.86	-35.67	70.23	15.00
110 TYR CB	-25.19	-34.54	69.43	15.00
110 TYR CG	-23.92	-34.95	68.76	15.00
110 TYR CD1	-22.72	-34.87	69.39	15.00
110 TYR CE1	-21.60	-35.34	68.80	15.00
110 TYR CD2	-23.95	-35.49	67.52	15.00
110 TYR CE2	-22.82	-35.97	66.92	15.00
110 TYR CZ	-21.64	-35.90	67.55	15.00
110 TYR OH	-20.45	-36.35	66.94	15.00
110 TYR C	-26.23	-36.85	69.29	15.00
110 TYR O	-25.46	-37.79	69.07	15.00
111 ARG N	-27.40	-36.72	68.69	15.00
111 ARG CA	-27.92	-37.70	67.75	15.00
111 ARG CB	-29.27	-38.26	68.26	15.00
111 ARG CG	-29.50	-39.79	68.03	15.00
111 ARG CD	-28.98	-40.22	66.68	15.00
111 ARG NE	-29.52	-41.47	66.17	15.00
111 ARG CZ	-30.81	-41.70	65.92	15.00
111 ARG NH1	-31.74	-40.77	66.15	15.00
111 ARG NH2	-31.18	-42.86	65.41	15.00
111 ARG C	-28.09	-37.07	66.36	15.00
111 ARG O	-28.58	-35.94	66.20	15.00
112 GLU N	-27.59	-37.78	65.36	15.00
112 GLU CA	-27.69	-37.35	63.96	15.00
112 GLU CB	-26.37	-37.55	63.21	15.00
112 GLU CG	-25.23	-36.68	63.74	15.00
112 GLU CD	-23.92	-36.94	63.06	15.00
112 GLU OE1	-23.53	-36.15	62.19	15.00
112 GLU OE2	-23.25	-37.90	63.42	15.00

TABLE VIII

112	GLU C	-28.84	-38.09	63.31	15.00
112	GLU O	-29.00	-39.31	63.50	15.00
113	ILE N	-29.66	-37.35	62.57	15.00
113	ILE CA	-30.83	-37.86	61.85	15.00
113	ILE CB	-31.89	-36.74	61.73	15.00
113	ILE CG2	-32.92	-37.06	60.63	15.00
113	ILE CG1	-32.57	-36.51	63.08	15.00
113	ILE CD1	-33.32	-35.23	63.13	15.00
113	ILE C	-30.46	-38.42	60.45	15.00
113	ILE O	-29.74	-37.79	59.70	15.00
114	PRO N	-30.93	-39.62	60.13	15.00
114	PRO CD	-31.77	-40.50	60.95	15.00
114	PRO CA	-30.66	-40.27	58.84	15.00
114	PRO CB	-31.85	-41.21	58.73	15.00
114	PRO CG	-31.86	-41.77	60.07	15.00
114	PRO C	-30.61	-39.34	57.65	15.00
114	PRO O	-31.62	-38.83	57.20	15.00
115	GLU N	-29.44	-39.26	57.05	15.00
115	GLU CA	-29.18	-38.44	55.87	15.00
115	GLU CB	-27.80	-38.78	55.30	15.00
115	GLU CG	-27.56	-38.41	53.84	15.00
115	GLU CD	-26.48	-39.24	53.21	15.00
115	GLU OE1	-26.78	-40.40	52.85	15.00
115	GLU OE2	-25.33	-38.75	53.12	15.00
115	GLU C	-30.20	-38.50	54.78	15.00
115	GLU O	-30.37	-39.53	54.16	15.00
116	GLY N	-30.90	-37.40	54.58	15.00
116	GLY CA	-31.88	-37.30	53.52	15.00
116	GLY C	-33.29	-37.78	53.79	15.00
116	GLY O	-34.11	-37.73	52.87	15.00
117	ASN N	-33.56	-38.25	55.01	15.00
117	ASN CA	-34.89	-38.73	55.36	15.00
117	ASN CB	-34.76	-40.00	56.22	15.00
117	ASN CG	-36.06	-40.77	56.33	15.00
117	ASN OD1	-37.13	-40.29	55.89	15.00
117	ASN ND2	-35.99	-41.96	56.91	15.00
117	ASN C	-35.76	-37.69	56.07	15.00
117	ASN O	-35.55	-37.38	57.23	15.00
118	GLU N	-36.72	-37.13	55.34	15.00
118	GLU CA	-37.65	-36.15	55.89	15.00
118	GLU CB	-38.29	-35.34	54.78	15.00
118	GLU CG	-37.31	-34.44	54.07	15.00
118	GLU CD	-38.00	-33.61	53.01	15.00

TABLE VIII

118 GLU OE1	-38.09	-34.08	51.85	15.00
118 GLU OE2	-38.48	-32.51	53.32	15.00
118 GLU C	-38.73	-36.78	56.75	15.00
118 GLU O	-39.42	-36.09	57.50	15.00
119 LYS N	-38.84	-38.11	56.68	15.00
119 LYS CA	-39.82	-38.82	57.49	15.00
119 LYS CB	-40.11	-40.20	56.91	15.00
119 LYS CG	-40.84	-41.15	57.86	15.00
119 LYS CD	-41.21	-42.46	57.19	15.00
119 LYS CE	-39.98	-43.29	56.80	15.00
119 LYS NZ	-38.99	-43.60	57.92	15.00
119 LYS C	-39.24	-38.95	58.88	15.00
119 LYS O	-39.97	-38.92	59.86	15.00
120 ALA N	-37.92	-39.06	58.95	15.00
120 ALA CA	-37.26	-39.21	60.24	15.00
120 ALA CB	-35.86	-39.73	60.05	15.00
120 ALA C	-37.20	-37.84	60.87	15.00
120 ALA O	-37.26	-37.70	62.09	15.00
121 LEU N	-37.08	-36.82	60.03	15.00
121 LEU CA	-36.98	-35.45	60.51	15.00
121 LEU CB	-36.44	-34.53	59.41	15.00
121 LEU CG	-36.17	-33.05	59.73	15.00
121 LEU CD1	-35.09	-32.86	60.74	15.00
121 LEU CD2	-35.74	-32.40	58.46	15.00
121 LEU C	-38.30	-34.95	61.07	15.00
121 LEU O	-38.33	-34.36	62.16	15.00
122 LYS N	-39.40	-35.27	60.39	15.00
122 LYS CA	-40.71	-34.88	60.89	15.00
122 LYS CB	-41.80	-35.31	59.90	15.00
122 LYS CG	-43.25	-35.03	60.34	15.00
122 LYS CD	-44.28	-35.77	59.47	15.00
122 LYS CE	-45.67	-35.70	60.08	15.00
122 LYS NZ	-46.60	-36.58	59.32	15.00
122 LYS C	-40.88	-35.54	62.26	15.00
122 LYS O	-41.33	-34.90	63.22	15.00
123 ARG N	-40.48	-36.81	62.38	15.00
123 ARG CA	-40.58	-37.50	63.65	15.00
123 ARG CB	-40.25	-38.98	63.52	15.00
123 ARG CG	-41.30	-39.84	62.88	15.00
123 ARG CD	-41.30	-41.21	63.51	15.00
123 ARG NE	-39.95	-41.78	63.60	15.00
123 ARG CZ	-39.25	-42.23	62.56	15.00
123 ARG NH1	-39.75	-42.19	61.32	15.00

TABLE VIII

123	ARG NH2	-38.05	-42.77	62.77	15.00
123	ARG C	-39.70	-36.88	64.73	15.00
123	ARG O	-40.18	-36.62	65.83	15.00
124	ALA N	-38.45	-36.57	64.41	15.00
124	ALA CA	-37.57	-35.99	65.43	15.00
124	ALA CB	-36.19	-35.74	64.86	15.00
124	ALA C	-38.12	-34.71	66.02	15.00
124	ALA O	-38.00	-34.46	67.22	15.00
125	VAL N	-38.77	-33.92	65.17	15.00
125	VAL CA	-39.36	-32.62	65.52	15.00
125	VAL CB	-39.54	-31.74	64.24	15.00
125	VAL CG1	-40.40	-30.50	64.54	15.00
125	VAL CG2	-38.15	-31.36	63.70	15.00
125	VAL C	-40.70	-32.75	66.24	15.00
125	VAL O	-41.14	-31.81	66.92	15.00
126	ALA N	-41.40	-33.85	66.02	15.00
126	ALA CA	-42.67	-34.05	66.68	15.00
126	ALA CB	-43.57	-35.00	65.86	15.00
126	ALA C	-42.42	-34.59	68.08	15.00
126	ALA O	-42.99	-34.11	69.06	15.00
127	ARG N	-41.47	-35.52	68.18	15.00
127	ARG CA	-41.15	-36.15	69.47	15.00
127	ARG CB	-40.71	-37.61	69.26	15.00
127	ARG CG	-41.77	-38.56	68.76	15.00
127	ARG CD	-42.88	-38.82	69.77	15.00
127	ARG NE	-43.75	-39.92	69.33	15.00
127	ARG CZ	-44.83	-40.35	69.98	15.00
127	ARG NH1	-45.54	-41.36	69.47	15.00
127	ARG NH2	-45.21	-39.78	71.13	15.00
127	ARG C	-40.13	-35.44	70.36	15.00
127	ARG O	-40.28	-35.42	71.58	15.00
128	VAL N	-39.07	-34.89	69.76	15.00
128	VAL CA	-37.97	-34.24	70.49	15.00
128	VAL CB	-36.63	-34.58	69.81	15.00
128	VAL CG1	-35.45	-34.03	70.61	15.00
128	VAL CG2	-36.48	-36.07	69.66	15.00
128	VAL C	-38.10	-32.73	70.56	15.00
128	VAL O	-37.92	-32.12	71.63	15.00
129	GLY N	-38.44	-32.14	69.42	15.00
129	GLY CA	-38.57	-30.70	69.33	15.00
129	GLY C	-37.60	-30.09	68.33	15.00
129	GLY O	-37.12	-30.79	67.45	15.00
130	PRO N	-37.31	-28.77	68.42	15.00

TABLE VIII

130	PRO	CD	-37.83	-27.89	69.47	15.00
130	PRO	CA	-36.40	-28.02	67.54	15.00
130	PRO	CB	-36.13	-26.77	68.34	15.00
130	PRO	CG	-37.40	-26.52	68.98	15.00
130	PRO	C	-35.13	-28.78	67.19	15.00
130	PRO	O	-34.38	-29.24	68.05	15.00
131	VAL	N	-34.91	-28.91	65.89	15.00
131	VAL	CA	-33.78	-29.63	65.37	15.00
131	VAL	CB	-34.27	-30.83	64.56	15.00
131	VAL	CG1	-33.10	-31.52	63.87	15.00
131	VAL	CG2	-35.02	-31.76	65.47	15.00
131	VAL	C	-32.91	-28.75	64.48	15.00
131	VAL	O	-33.43	-28.02	63.65	15.00
132	SER	N	-31.60	-28.85	64.68	15.00
132	SER	CA	-30.59	-28.13	63.91	15.00
132	SER	CB	-29.21	-28.32	64.54	15.00
132	SER	OG	-28.89	-27.37	65.52	15.00
132	SER	C	-30.50	-28.73	62.50	15.00
132	SER	O	-30.34	-29.94	62.34	15.00
133	VAL	N	-30.47	-27.87	61.50	15.00
133	VAL	CA	-30.38	-28.36	60.13	15.00
133	VAL	CB	-31.75	-28.35	59.45	15.00
133	VAL	CG1	-32.73	-29.24	60.17	15.00
133	VAL	CG2	-32.30	-26.98	59.41	15.00
133	VAL	C	-29.52	-27.41	59.35	15.00
133	VAL	O	-29.29	-26.29	59.79	15.00
134	ALA	N	-29.14	-27.85	58.15	15.00
134	ALA	CA	-28.32	-27.08	57.22	15.00
134	ALA	CB	-26.99	-27.75	56.97	15.00
134	ALA	C	-29.14	-27.06	55.95	15.00
134	ALA	O	-29.99	-27.92	55.71	15.00
135	ILE	N	-28.79	-26.11	55.09	15.00
135	ILE	CA	-29.49	-25.93	53.83	15.00
135	ILE	CB	-30.82	-25.12	54.04	15.00
135	ILE	CG2	-31.90	-26.00	54.64	15.00
135	ILE	CG1	-30.57	-23.83	54.85	15.00
135	ILE	CD1	-31.76	-22.91	54.86	15.00
135	ILE	C	-28.69	-25.16	52.82	15.00
135	ILE	O	-27.58	-24.73	53.10	15.00
136	ASP	N	-29.20	-25.10	51.61	15.00
136	ASP	CA	-28.56	-24.32	50.56	15.00
136	ASP	CB	-28.74	-24.95	49.18	15.00
136	ASP	CG	-28.23	-24.06	48.08	15.00

TABLE VIII

136 ASP OD1	-28.28	-24.45	46.91	15.00
136 ASP OD2	-27.73	-22.96	48.35	15.00
136 ASP C	-29.32	-23.01	50.62	15.00
136 ASP O	-30.51	-22.93	50.35	15.00
137 ALA N	-28.59	-21.94	50.84	15.00
137 ALA CA	-29.23	-20.64	50.97	15.00
137 ALA CB	-29.22	-20.22	52.43	15.00
137 ALA C	-28.65	-19.55	50.07	15.00
137 ALA O	-28.89	-18.38	50.30	15.00
138 SER N	-27.97	-19.97	49.00	15.00
138 SER CA	-27.34	-19.06	48.03	15.00
138 SER CB	-26.28	-19.80	47.23	15.00
138 SER OG	-26.71	-21.14	47.02	15.00
138 SER C	-28.32	-18.41	47.07	15.00
138 SER O	-28.09	-17.29	46.57	15.00
139 LEU N	-29.42	-19.14	46.81	15.00
139 LEU CA	-30.44	-18.68	45.87	15.00
139 LEU CB	-31.60	-19.68	45.83	15.00
139 LEU CG	-31.57	-20.77	44.76	15.00
139 LEU CD1	-31.68	-20.14	43.39	15.00
139 LEU CD2	-30.29	-21.58	44.84	15.00
139 LEU C	-30.95	-17.30	46.25	15.00
139 LEU O	-31.39	-17.09	47.37	15.00
140 THR N	-30.99	-16.39	45.28	15.00
140 THR CA	-31.41	-15.04	45.54	15.00
140 THR CB	-31.16	-14.10	44.30	15.00
140 THR OG1	-30.83	-14.87	43.13	15.00
140 THR CG2	-30.00	-13.22	44.59	15.00
140 THR C	-32.86	-14.97	46.00	15.00
140 THR O	-33.25	-14.00	46.66	15.00
141 SER N	-33.65	-15.99	45.68	15.00
141 SER CA	-35.05	-16.03	46.09	15.00
141 SER CB	-35.80	-17.14	45.35	15.00
141 SER OG	-34.95	-18.27	45.17	15.00
141 SER C	-35.15	-16.16	47.60	15.00
141 SER O	-35.95	-15.48	48.25	15.00
142 PHE N	-34.23	-16.95	48.15	15.00
142 PHE CA	-34.11	-17.19	49.58	15.00
142 PHE CB	-32.92	-18.13	49.84	15.00
142 PHE CG	-32.94	-18.73	51.21	15.00
142 PHE CD1	-33.41	-20.03	51.41	15.00
142 PHE CD2	-32.54	-17.97	52.34	15.00
142 PHE CE1	-33.50	-20.55	52.67	15.00

TABLE VIII

142	PHE	CE2	-32.63	-18.49	53.60	15.00
142	PHE	CZ	-33.10	-19.77	53.78	15.00
142	PHE	C	-33.90	-15.87	50.34	15.00
142	PHE	O	-34.57	-15.60	51.33	15.00
143	GLN	N	-33.02	-15.01	49.84	15.00
143	GLN	CA	-32.74	-13.74	50.49	15.00
143	GLN	CB	-31.45	-13.14	49.95	15.00
143	GLN	CG	-30.34	-14.15	49.75	15.00
143	GLN	CD	-29.07	-13.49	49.24	15.00
143	GLN	OE1	-29.02	-12.26	49.08	15.00
143	GLN	NE2	-28.02	-14.29	49.00	15.00
143	GLN	C	-33.90	-12.76	50.35	15.00
143	GLN	O	-34.20	-12.02	51.29	15.00
144	PHE	N	-34.58	-12.77	49.20	15.00
144	PHE	CA	-35.72	-11.87	49.00	15.00
144	PHE	CB	-35.76	-11.31	47.56	15.00
144	PHE	CG	-34.56	-10.48	47.21	15.00
144	PHE	CD1	-34.12	-9.49	48.08	15.00
144	PHE	CD2	-33.89	-10.69	46.02	15.00
144	PHE	CE1	-33.03	-8.71	47.77	15.00
144	PHE	CE2	-32.80	-9.92	45.68	15.00
144	PHE	CZ	-32.36	-8.93	46.55	15.00
144	PHE	C	-37.07	-12.48	49.36	15.00
144	PHE	O	-38.09	-11.81	49.24	15.00
145	TYR	N	-37.08	-13.74	49.80	15.00
145	TYR	CA	-38.31	-14.45	50.22	15.00
145	TYR	CB	-37.94	-15.77	50.96	15.00
145	TYR	CG	-39.07	-16.36	51.80	15.00
145	TYR	CD1	-39.94	-17.34	51.29	15.00
145	TYR	CE1	-41.00	-17.82	52.05	15.00
145	TYR	CD2	-39.30	-15.88	53.10	15.00
145	TYR	CE2	-40.33	-16.32	53.86	15.00
145	TYR	CZ	-41.19	-17.29	53.34	15.00
145	TYR	OH	-42.25	-17.67	54.16	15.00
145	TYR	C	-39.14	-13.55	51.14	15.00
145	TYR	O	-38.60	-12.81	51.97	15.00
146	SER	N	-40.45	-13.64	51.02	15.00
146	SER	CA	-41.31	-12.83	51.88	15.00
146	SER	CB	-41.74	-11.55	51.16	15.00
146	SER	OG	-40.94	-10.40	51.51	15.00
146	SER	C	-42.53	-13.55	52.45	15.00
146	SER	O	-42.89	-13.33	53.61	15.00
147	LYS	N	-43.15	-14.44	51.68	15.00

TABLE VIII

147	LYS	CA	-44.33	-15.12	52.17	15.00
147	LYS	CB	-45.53	-14.22	51.94	15.00
147	LYS	CG	-45.80	-13.23	53.02	15.00
147	LYS	CD	-46.76	-12.13	52.55	15.00
147	LYS	CE	-47.91	-12.66	51.67	15.00
147	LYS	NZ	-48.65	-13.77	52.35	15.00
147	LYS	C	-44.63	-16.41	51.41	15.00
147	LYS	O	-44.45	-16.45	50.20	15.00
148	GLY	N	-45.09	-17.43	52.10	15.00
148	GLY	CA	-45.45	-18.66	51.42	15.00
148	GLY	C	-44.53	-19.82	51.65	15.00
148	GLY	O	-43.56	-19.73	52.41	15.00
149	VAL	N	-44.79	-20.91	50.92	15.00
149	VAL	CA	-43.99	-22.13	50.98	15.00
149	VAL	CB	-44.85	-23.39	50.69	15.00
149	VAL	CG1	-43.98	-24.66	50.78	15.00
149	VAL	CG2	-45.98	-23.43	51.62	15.00
149	VAL	C	-42.91	-22.02	49.90	15.00
149	VAL	O	-43.22	-22.06	48.72	15.00
150	TYR	N	-41.68	-21.79	50.34	15.00
150	TYR	CA	-40.49	-21.66	49.49	15.00
150	TYR	CB	-39.31	-21.17	50.33	15.00
150	TYR	CG	-38.07	-21.02	49.48	15.00
150	TYR	CD1	-37.90	-19.91	48.65	15.00
150	TYR	CE1	-36.75	-19.75	47.90	15.00
150	TYR	CD2	-37.05	-21.97	49.52	15.00
150	TYR	CE2	-35.89	-21.82	48.77	15.00
150	TYR	CZ	-35.75	-20.71	47.97	15.00
150	TYR	OH	-34.59	-20.55	47.26	15.00
150	TYR	C	-40.04	-22.89	48.73	15.00
150	TYR	O	-39.72	-23.95	49.29	15.00
151	TYR	N	-39.88	-22.68	47.44	15.00
151	TYR	CA	-39.46	-23.73	46.54	15.00
151	TYR	CB	-40.63	-24.64	46.18	15.00
151	TYR	CG	-40.18	-25.91	45.48	15.00
151	TYR	CD1	-39.56	-26.99	46.24	15.00
151	TYR	CE1	-39.05	-28.12	45.59	15.00
151	TYR	CD2	-40.31	-25.99	44.05	15.00
151	TYR	CE2	-39.83	-27.07	43.37	15.00
151	TYR	CZ	-39.19	-28.15	44.13	15.00
151	TYR	OH	-38.66	-29.25	43.41	15.00
151	TYR	C	-38.86	-23.09	45.29	15.00
151	TYR	O	-39.45	-22.21	44.68	15.00

TABLE VIII

152 ASP N	-37.66	-23.52	44.96	15.00
152 ASP CA	-36.90	-23.04	43.81	15.00
152 ASP CB	-35.90	-21.97	44.26	15.00
152 ASP CG	-35.26	-21.25	43.08	15.00
152 ASP OD1	-35.42	-20.01	42.99	15.00
152 ASP OD2	-34.63	-21.92	42.23	15.00
152 ASP C	-36.16	-24.28	43.31	15.00
152 ASP O	-35.56	-25.00	44.09	15.00
153 GLU N	-36.16	-24.49	42.00	15.00
153 GLU CA	-35.56	-25.67	41.38	15.00
153 GLU CB	-36.09	-25.74	39.97	15.00
153 GLU CG	-35.94	-24.42	39.26	15.00
153 GLU CD	-36.44	-24.48	37.83	15.00
153 GLU OE1	-35.63	-24.12	36.94	15.00
153 GLU OE2	-37.62	-24.87	37.62	15.00
153 GLU C	-34.04	-25.70	41.31	15.00
153 GLU O	-33.47	-26.73	40.99	15.00
154 SER N	-33.39	-24.59	41.60	15.00
154 SER CA	-31.95	-24.48	41.56	15.00
154 SER CB	-31.59	-23.07	41.09	15.00
154 SER OG	-32.22	-22.78	39.85	15.00
154 SER C	-31.28	-24.79	42.91	15.00
154 SER O	-30.07	-24.67	43.03	15.00
155 CYS N	-32.08	-25.19	43.90	15.00
155 CYS CA	-31.55	-25.49	45.23	15.00
155 CYS C	-30.88	-26.84	45.21	15.00
155 CYS O	-31.52	-27.87	45.08	15.00
155 CYS CB	-32.63	-25.43	46.33	15.00
155 CYS SG	-32.25	-24.44	47.82	15.00
156 ASN N	-29.57	-26.79	45.39	15.00
156 ASN CA	-28.70	-27.97	45.38	15.00
156 ASN CB	-27.30	-27.52	44.99	15.00
156 ASN CG	-26.51	-28.59	44.35	15.00
156 ASN OD1	-26.70	-29.78	44.62	15.00
156 ASN ND2	-25.58	-28.18	43.51	15.00
156 ASN C	-28.63	-28.71	46.72	15.00
156 ASN O	-28.12	-28.19	47.70	15.00
157 SER N	-29.09	-29.96	46.73	15.00
157 SER CA	-29.09	-30.77	47.95	15.00
157 SER CB	-29.77	-32.11	47.70	15.00
157 SER OG	-31.03	-31.95	47.10	15.00
157 SER C	-27.68	-31.08	48.43	15.00
157 SER O	-27.48	-31.52	49.54	15.00

TABLE VIII

158 ASP N	-26.71	-30.93	47.55	15.00
158 ASP CA	-25.34	-31.23	47.91	15.00
158 ASP CB	-24.69	-32.07	46.78	15.00
158 ASP CG	-25.32	-33.44	46.67	15.00
158 ASP OD1	-26.15	-33.63	45.75	15.00
158 ASP OD2	-25.05	-34.30	47.55	15.00
158 ASP C	-24.46	-30.07	48.28	15.00
158 ASP O	-23.27	-30.25	48.57	15.00
159 ASN N	-25.05	-28.88	48.29	15.00
159 ASN CA	-24.30	-27.69	48.61	15.00
159 ASN CB	-24.34	-26.74	47.42	15.00
159 ASN CG	-23.51	-25.49	47.62	15.00
159 ASN OD1	-22.35	-25.55	48.00	15.00
159 ASN ND2	-24.12	-24.33	47.38	15.00
159 ASN C	-24.93	-27.03	49.82	15.00
159 ASN O	-25.67	-26.05	49.68	15.00
160 LEU N	-24.68	-27.59	50.99	15.00
160 LEU CA	-25.16	-27.07	52.24	15.00
160 LEU CB	-25.06	-28.15	53.29	15.00
160 LEU CG	-25.72	-29.45	52.83	15.00
160 LEU CD1	-25.24	-30.64	53.62	15.00
160 LEU CD2	-27.22	-29.26	52.91	15.00
160 LEU C	-24.22	-25.95	52.63	15.00
160 LEU O	-23.06	-26.21	52.92	15.00
161 ASN N	-24.73	-24.74	52.74	15.00
161 ASN CA	-23.91	-23.58	53.10	15.00
161 ASN CB	-23.61	-22.78	51.83	15.00
161 ASN CG	-24.84	-22.55	50.93	15.00
161 ASN OD1	-25.71	-21.74	51.22	15.00
161 ASN ND2	-24.92	-23.31	49.84	15.00
161 ASN C	-24.42	-22.67	54.23	15.00
161 ASN O	-23.75	-21.70	54.59	15.00
162 HIS N	-25.60	-22.96	54.76	15.00
162 HIS CA	-26.13	-22.19	55.86	15.00
162 HIS CB	-27.12	-21.15	55.35	15.00
162 HIS CG	-27.63	-20.21	56.41	15.00
162 HIS CD2	-28.89	-19.99	56.84	15.00
162 HIS ND1	-26.82	-19.39	57.16	15.00
162 HIS CE1	-27.56	-18.68	57.99	15.00
162 HIS NE2	-28.82	-19.03	57.82	15.00
162 HIS C	-26.80	-23.11	56.86	15.00
162 HIS O	-27.41	-24.10	56.49	15.00
163 ALA N	-26.61	-22.84	58.14	15.00

163	ALA	CA	-27.27	-23.63	59.17	15.00
163	ALA	CB	-26.35	-23.90	60.32	15.00
163	ALA	C	-28.47	-22.85	59.65	15.00
163	ALA	O	-28.43	-21.62	59.83	15.00
164	VAL	N	-29.53	-23.57	59.97	15.00
164	VAL	CA	-30.75	-22.92	60.40	15.00
164	VAL	CB	-31.54	-22.58	59.10	15.00
164	VAL	CG1	-32.42	-23.71	58.68	15.00
164	VAL	CG2	-32.27	-21.27	59.22	15.00
164	VAL	C	-31.49	-23.77	61.47	15.00
164	VAL	O	-31.01	-24.81	61.87	15.00
165	LEU	N	-32.64	-23.32	61.97	15.00
165	LEU	CA	-33.33	-24.10	62.98	15.00
165	LEU	CB	-33.27	-23.41	64.32	15.00
165	LEU	CG	-33.72	-24.12	65.58	15.00
165	LEU	CD1	-32.59	-24.89	66.21	15.00
165	LEU	CD2	-34.18	-23.05	66.52	15.00
165	LEU	C	-34.76	-24.44	62.63	15.00
165	LEU	O	-35.55	-23.56	62.28	15.00
166	ALA	N	-35.05	-25.73	62.66	15.00
166	ALA	CA	-36.37	-26.25	62.37	15.00
166	ALA	CB	-36.25	-27.61	61.71	15.00
166	ALA	C	-37.09	-26.35	63.69	15.00
166	ALA	O	-36.63	-27.02	64.62	15.00
167	VAL	N	-38.24	-25.69	63.76	15.00
167	VAL	CA	-39.08	-25.64	64.97	15.00
167	VAL	CB	-39.16	-24.22	65.61	15.00
167	VAL	CG1	-37.79	-23.68	65.96	15.00
167	VAL	CG2	-39.89	-23.25	64.67	15.00
167	VAL	C	-40.52	-26.07	64.76	15.00
167	VAL	O	-41.40	-25.61	65.46	15.00
168	GLY	N	-40.78	-26.91	63.77	15.00
168	GLY	CA	-42.15	-27.34	63.56	15.00
168	GLY	C	-42.35	-27.62	62.09	15.00
168	GLY	O	-41.42	-27.58	61.31	15.00
169	TYR	N	-43.58	-27.95	61.73	15.00
169	TYR	CA	-43.99	-28.29	60.36	15.00
169	TYR	CB	-43.51	-29.71	59.99	15.00
169	TYR	CG	-44.07	-30.82	60.89	15.00
169	TYR	CD1	-45.33	-31.41	60.61	15.00
169	TYR	CE1	-45.86	-32.39	61.43	15.00
169	TYR	CD2	-43.34	-31.27	62.02	15.00
169	TYR	CE2	-43.88	-32.28	62.86	15.00

169 TYR CZ	-45.12	-32.81	62.55	15.00
169 TYR OH	-45.63	-33.71	63.41	15.00
169 TYR C	-45.53	-28.26	60.32	15.00
169 TYR O	-46.20	-28.25	61.37	15.00
170 GLY N	-46.09	-28.23	59.12	15.00
170 GLY CA	-47.54	-28.17	58.95	15.00
170 GLY C	-47.93	-28.06	57.48	15.00
170 GLY O	-47.12	-28.35	56.61	15.00
171 ILE N	-49.14	-27.61	57.17	15.00
171 ILE CA	-49.55	-27.54	55.77	15.00
171 ILE CB	-50.30	-28.85	55.41	15.00
171 ILE CG2	-51.37	-29.17	56.40	15.00
171 ILE CG1	-50.79	-28.82	53.99	15.00
171 ILE CD1	-51.11	-30.20	53.45	15.00
171 ILE C	-50.38	-26.29	55.43	15.00
171 ILE O	-51.37	-26.02	56.10	15.00
172 GLN N	-49.93	-25.52	54.44	15.00
172 GLN CA	-50.64	-24.31	54.01	15.00
172 GLN CB	-49.68	-23.10	54.05	15.00
172 GLN CG	-50.30	-21.69	53.87	15.00
172 GLN CD	-49.27	-20.56	53.75	15.00
172 GLN OE1	-48.07	-20.77	53.89	15.00
172 GLN NE2	-49.74	-19.35	53.49	15.00
172 GLN C	-51.25	-24.41	52.63	15.00
172 GLN O	-50.56	-24.19	51.64	15.00
173 LYS N	-52.55	-24.75	52.57	15.00
173 LYS CA	-53.33	-24.85	51.32	15.00
173 LYS CB	-53.40	-23.48	50.61	15.00
173 LYS CG	-54.16	-22.39	51.36	15.00
173 LYS CD	-53.57	-22.02	52.75	15.00
173 LYS CE	-54.37	-22.65	53.92	15.00
173 LYS NZ	-54.04	-22.06	55.23	15.00
173 LYS C	-52.85	-25.93	50.36	15.00
173 LYS O	-52.73	-25.69	49.15	15.00
174 GLY N	-52.61	-27.11	50.90	15.00
174 GLY CA	-52.15	-28.21	50.08	15.00
174 GLY C	-50.64	-28.26	50.03	15.00
174 GLY O	-50.08	-29.23	49.53	15.00
175 ASN N	-49.97	-27.25	50.58	15.00
175 ASN CA	-48.52	-27.27	50.57	15.00
175 ASN CB	-47.92	-26.00	49.95	15.00
175 ASN CG	-48.48	-25.73	48.57	15.00
175 ASN OD1	-48.53	-26.61	47.73	15.00

175 ASN ND2	-48.96	-24.51	48.37	15.00
175 ASN C	-47.94	-27.50	51.94	15.00
175 ASN O	-48.04	-26.66	52.86	15.00
176 LYS N	-47.37	-28.69	52.07	15.00
176 LYS CA	-46.71	-29.13	53.27	15.00
176 LYS CB	-46.28	-30.61	53.08	15.00
176 LYS CG	-47.40	-31.59	52.68	15.00
176 LYS CD	-47.20	-32.92	53.41	15.00
176 LYS CE	-48.36	-33.85	53.17	15.00
176 LYS NZ	-48.49	-34.80	54.30	15.00
176 LYS C	-45.51	-28.18	53.48	15.00
176 LYS O	-45.12	-27.49	52.55	15.00
177 HIS N	-44.94	-28.15	54.68	15.00
177 HIS CA	-43.82	-27.26	54.97	15.00
177 HIS CB	-44.23	-25.79	54.78	15.00
177 HIS CG	-45.19	-25.25	55.82	15.00
177 HIS CD2	-45.07	-25.11	57.17	15.00
177 HIS ND1	-46.37	-24.62	55.49	15.00
177 HIS CE1	-46.93	-24.11	56.58	15.00
177 HIS NE2	-46.16	-24.40	57.61	15.00
177 HIS C	-43.08	-27.42	56.30	15.00
177 HIS O	-43.62	-27.92	57.28	15.00
178 TRP N	-41.81	-27.01	56.29	15.00
178 TRP CA	-40.97	-27.01	57.48	15.00
178 TRP CB	-39.52	-27.41	57.16	15.00
178 TRP CG	-39.34	-28.83	56.89	15.00
178 TRP CD2	-39.46	-29.91	57.82	15.00
178 TRP CE2	-39.29	-31.11	57.09	15.00
178 TRP CE3	-39.70	-29.97	59.20	15.00
178 TRP CD1	-39.09	-29.39	55.68	15.00
178 TRP NE1	-39.07	-30.76	55.78	15.00
178 TRP CZ2	-39.34	-32.38	57.67	15.00
178 TRP CZ3	-39.76	-31.22	59.78	15.00
178 TRP CH2	-39.58	-32.42	59.01	15.00
178 TRP C	-41.00	-25.55	57.95	15.00
178 TRP O	-41.12	-24.64	57.14	15.00
179 ILE N	-41.04	-25.34	59.26	15.00
179 ILE CA	-41.05	-23.98	59.78	15.00
179 ILE CB	-41.99	-23.89	60.97	15.00
179 ILE CG2	-41.90	-22.54	61.61	15.00
179 ILE CG1	-43.42	-24.18	60.51	15.00
179 ILE CD1	-44.37	-24.29	61.63	15.00
179 ILE C	-39.62	-23.75	60.20	15.00

179	ILE O	-39.07	-24.45	61.07	15.00
180	ILE N	-38.99	-22.78	59.57	15.00
180	ILE CA	-37.58	-22.52	59.86	15.00
180	ILE CB	-36.79	-22.59	58.57	15.00
180	ILE CG2	-35.36	-22.38	58.83	15.00
180	ILE CG1	-36.99	-23.93	57.91	15.00
180	ILE CD1	-36.41	-25.01	58.75	15.00
180	ILE C	-37.25	-21.18	60.52	15.00
180	ILE O	-37.82	-20.13	60.17	15.00
181	LYS N	-36.35	-21.19	61.49	15.00
181	LYS CA	-35.97	-19.95	62.16	15.00
181	LYS CB	-35.83	-20.19	63.65	15.00
181	LYS CG	-35.49	-18.92	64.45	15.00
181	LYS CD	-35.36	-19.25	65.93	15.00
181	LYS CE	-35.01	-18.04	66.76	15.00
181	LYS NZ	-34.86	-18.51	68.16	15.00
181	LYS C	-34.64	-19.50	61.61	15.00
181	LYS O	-33.72	-20.32	61.54	15.00
182	ASN N	-34.49	-18.23	61.27	15.00
182	ASN CA	-33.22	-17.79	60.71	15.00
182	ASN CB	-33.45	-17.10	59.34	15.00
182	ASN CG	-32.32	-17.37	58.34	15.00
182	ASN OD1	-31.30	-18.02	58.65	15.00
182	ASN ND2	-32.53	-16.89	57.09	15.00
182	ASN C	-32.54	-16.84	61.68	15.00
182	ASN O	-33.16	-16.31	62.60	15.00
183	SER N	-31.25	-16.64	61.45	15.00
183	SER CA	-30.40	-15.74	62.23	15.00
183	SER CB	-29.16	-16.50	62.75	15.00
183	SER OG	-28.52	-17.33	61.76	15.00
183	SER C	-29.95	-14.52	61.41	15.00
183	SER O	-28.81	-14.06	61.56	15.00
184	TRP N	-30.82	-13.98	60.55	15.00
184	TRP CA	-30.50	-12.82	59.71	15.00
184	TRP CB	-30.71	-13.10	58.22	15.00
184	TRP CG	-29.79	-14.06	57.58	15.00
184	TRP CD2	-29.90	-14.58	56.26	15.00
184	TRP CE2	-28.80	-15.45	56.05	15.00
184	TRP CE3	-30.82	-14.38	55.22	15.00
184	TRP CD1	-28.66	-14.61	58.11	15.00
184	TRP NE1	-28.06	-15.46	57.20	15.00
184	TRP CZ2	-28.59	-16.14	54.84	15.00
184	TRP CZ3	-30.63	-15.04	54.04	15.00

184 TRP CH2	-29.52	-15.92	53.84	15.00
184 TRP C	-31.34	-11.59	60.02	15.00
184 TRP O	-31.41	-10.70	59.18	15.00
185 GLY N	-31.95	-11.51	61.20	15.00
185 GLY CA	-32.75	-10.34	61.52	15.00
185 GLY C	-34.24	-10.61	61.41	15.00
185 GLY O	-34.63	-11.61	60.82	15.00
186 GLU N	-35.09	-9.75	61.96	15.00
186 GLU CA	-36.52	-10.00	61.83	15.00
186 GLU CB	-37.32	-9.44	63.01	15.00
186 GLU CG	-36.65	-9.45	64.34	15.00
186 GLU CD	-37.34	-8.56	65.32	15.00
186 GLU OE1	-36.68	-8.08	66.25	15.00
186 GLU OE2	-38.55	-8.32	65.21	15.00
186 GLU C	-36.99	-9.30	60.56	15.00
186 GLU O	-38.10	-9.52	60.08	15.00
187 ASN N	-36.14	-8.44	60.02	15.00
187 ASN CA	-36.46	-7.68	58.83	15.00
187 ASN CB	-35.60	-6.42	58.79	15.00
187 ASN CG	-35.84	-5.51	59.97	15.00
187 ASN OD1	-34.92	-4.82	60.44	15.00
187 ASN ND2	-37.10	-5.46	60.45	15.00
187 ASN C	-36.21	-8.52	57.60	15.00
187 ASN O	-36.21	-8.00	56.49	15.00
188 TRP N	-35.89	-9.79	57.81	15.00
188 TRP CA	-35.66	-10.68	56.68	15.00
188 TRP CB	-34.39	-11.49	56.84	15.00
188 TRP CG	-34.20	-12.53	55.78	15.00
188 TRP CD2	-34.69	-13.89	55.77	15.00
188 TRP CE2	-34.21	-14.49	54.59	15.00
188 TRP CE3	-35.48	-14.67	56.67	15.00
188 TRP CD1	-33.48	-12.37	54.63	15.00
188 TRP NE1	-33.48	-13.54	53.91	15.00
188 TRP CZ2	-34.50	-15.83	54.26	15.00
188 TRP CZ3	-35.76	-15.96	56.35	15.00
188 TRP CH2	-35.28	-16.55	55.16	15.00
188 TRP C	-36.80	-11.63	56.71	15.00
188 TRP O	-37.29	-11.96	57.78	15.00
189 GLY N	-37.22	-12.09	55.53	15.00
189 GLY CA	-38.30	-13.05	55.42	15.00
189 GLY C	-39.53	-12.66	56.18	15.00
189 GLY O	-39.85	-11.50	56.32	15.00
190 ASN N	-40.23	-13.64	56.73	15.00

190 ASN CA	-41.43	-13.31	57.46	15.00
190 ASN CB	-42.42	-14.44	57.30	15.00
190 ASN CG	-43.81	-14.05	57.76	15.00
190 ASN OD1	-44.10	-12.89	58.14	15.00
190 ASN ND2	-44.72	-15.00	57.62	15.00
190 ASN C	-41.04	-13.20	58.90	15.00
190 ASN O	-40.92	-14.22	59.57	15.00
191 LYS N	-40.80	-11.98	59.38	15.00
191 LYS CA	-40.39	-11.79	60.76	15.00
191 LYS CB	-41.62	-11.71	61.67	15.00
191 LYS CG	-42.53	-10.45	61.51	15.00
191 LYS CD	-43.64	-10.73	60.48	15.00
191 LYS CE	-44.65	-9.57	60.22	15.00
191 LYS NZ	-44.60	-8.96	58.86	15.00
191 LYS C	-39.36	-12.83	61.26	15.00
191 LYS O	-39.58	-13.50	62.27	15.00
192 GLY N	-38.25	-12.96	60.52	15.00
192 GLY CA	-37.17	-13.89	60.87	15.00
192 GLY C	-37.47	-15.35	60.56	15.00
192 GLY O	-36.64	-16.20	60.86	15.00
193 TYR N	-38.59	-15.63	59.91	15.00
193 TYR CA	-38.89	-17.04	59.63	15.00
193 TYR CB	-40.12	-17.53	60.44	15.00
193 TYR CG	-39.91	-17.72	61.94	15.00
193 TYR CD1	-39.96	-16.63	62.83	15.00
193 TYR CE1	-39.79	-16.81	64.19	15.00
193 TYR CD2	-39.69	-18.99	62.47	15.00
193 TYR CE2	-39.52	-19.20	63.79	15.00
193 TYR CZ	-39.56	-18.12	64.67	15.00
193 TYR OH	-39.33	-18.34	66.03	15.00
193 TYR C	-39.11	-17.29	58.14	15.00
193 TYR O	-39.23	-16.35	57.35	15.00
194 ILE N	-39.08	-18.56	57.75	15.00
194 ILE CA	-39.32	-18.92	56.37	15.00
194 ILE CB	-37.98	-18.83	55.52	15.00
194 ILE CG2	-36.90	-19.78	56.01	15.00
194 ILE CG1	-38.23	-19.04	54.02	15.00
194 ILE CD1	-36.98	-19.00	53.22	15.00
194 ILE C	-39.99	-20.30	56.33	15.00
194 ILE O	-39.67	-21.15	57.18	15.00
195 LEU N	-41.01	-20.45	55.48	15.00
195 LEU CA	-41.71	-21.72	55.30	15.00
195 LEU CB	-43.20	-21.48	55.00	15.00

195 LEU CG	-43.96	-20.94	56.22	15.00
195 LEU CD1	-45.35	-20.46	55.85	15.00
195 LEU CD2	-44.03	-22.03	57.28	15.00
195 LEU C	-41.08	-22.46	54.14	15.00
195 LEU O	-41.24	-22.03	52.99	15.00
196 MET N	-40.38	-23.55	54.41	15.00
196 MET CA	-39.73	-24.28	53.34	15.00
196 MET CB	-38.30	-24.61	53.74	15.00
196 MET CG	-37.40	-23.37	53.79	15.00
196 MET SD	-35.72	-23.74	54.33	15.00
196 MET CE	-35.19	-24.86	53.02	15.00
196 MET C	-40.45	-25.54	52.91	15.00
196 MET O	-40.92	-26.29	53.76	15.00
197 ALA N	-40.52	-25.77	51.61	15.00
197 ALA CA	-41.19	-26.95	51.06	15.00
197 ALA CB	-40.98	-26.99	49.58	15.00
197 ALA C	-40.77	-28.28	51.69	15.00
197 ALA O	-39.59	-28.51	51.93	15.00
198 ARG N	-41.77	-29.13	51.96	15.00
198 ARG CA	-41.53	-30.45	52.55	15.00
198 ARG CB	-42.18	-30.53	53.94	15.00
198 ARG CG	-42.26	-31.94	54.56	15.00
198 ARG CD	-42.45	-31.86	56.05	15.00
198 ARG NE	-43.59	-31.03	56.41	15.00
198 ARG CZ	-44.85	-31.46	56.47	15.00
198 ARG NH1	-45.11	-32.72	56.19	15.00
198 ARG NH2	-45.84	-30.65	56.84	15.00
198 ARG C	-42.05	-31.55	51.67	15.00
198 ARG O	-43.07	-31.41	50.99	15.00
199 ASN N	-41.39	-32.69	51.77	15.00
199 ASN CA	-41.70	-33.89	51.02	15.00
199 ASN CB	-43.17	-34.27	51.14	15.00
199 ASN CG	-43.54	-34.74	52.54	15.00
199 ASN OD1	-42.66	-34.97	53.39	15.00
199 ASN ND2	-44.84	-34.86	52.79	15.00
199 ASN C	-41.32	-33.73	49.56	15.00
199 ASN O	-41.24	-34.72	48.84	15.00
200 LYS N	-41.04	-32.51	49.14	15.00
200 LYS CA	-40.66	-32.31	47.77	15.00
200 LYS CB	-40.98	-30.88	47.33	15.00
200 LYS CG	-42.41	-30.50	47.40	15.00
200 LYS CD	-42.69	-29.14	46.77	15.00
200 LYS CE	-42.63	-29.16	45.28	15.00

200	LYS	NZ	-43.85	-29.82	44.77	15.00
200	LYS	C	-39.20	-32.67	47.45	15.00
200	LYS	O	-38.40	-31.81	47.09	15.00
201	ASN	N	-38.85	-33.95	47.62	15.00
201	ASN	CA	-37.50	-34.49	47.34	15.00
201	ASN	CB	-37.30	-34.62	45.82	15.00
201	ASN	CG	-38.27	-35.59	45.16	15.00
201	ASN	OD1	-37.88	-36.36	44.27	15.00
201	ASN	ND2	-39.56	-35.52	45.54	15.00
201	ASN	C	-36.34	-33.71	47.95	15.00
201	ASN	O	-35.58	-33.08	47.22	15.00
202	ASN	N	-36.22	-33.75	49.28	15.00
202	ASN	CA	-35.14	-33.08	50.02	15.00
202	ASN	CB	-33.88	-33.93	49.92	15.00
202	ASN	CG	-33.05	-33.91	51.18	15.00
202	ASN	OD1	-33.57	-33.92	52.30	15.00
202	ASN	ND2	-31.73	-33.90	51.01	15.00
202	ASN	C	-34.85	-31.68	49.53	15.00
202	ASN	O	-33.72	-31.35	49.20	15.00
203	ALA	N	-35.85	-30.82	49.54	15.00
203	ALA	H	-36.60	-31.08	50.11	15.00
203	ALA	CA	-35.72	-29.46	49.02	15.00
203	ALA	CB	-36.91	-28.60	49.43	15.00
203	ALA	C	-34.46	-28.80	49.61	15.00
203	ALA	O	-34.31	-28.70	50.79	15.00
204	CYS	N	-33.59	-28.31	48.74	15.00
204	CYS	CA	-32.40	-27.62	49.21	15.00
204	CYS	C	-31.47	-28.47	50.07	15.00
204	CYS	O	-30.40	-28.02	50.45	15.00
204	CYS	CB	-32.76	-26.38	50.00	15.00
204	CYS	SG	-33.64	-25.09	49.12	15.00
205	GLY	N	-31.91	-29.64	50.49	15.00
205	GLY	CA	-31.04	-30.48	51.28	15.00
205	GLY	C	-31.30	-30.32	52.77	15.00
205	GLY	O	-30.40	-30.54	53.58	15.00
206	ILE	N	-32.52	-29.94	53.13	15.00
206	ILE	CA	-32.90	-29.75	54.52	15.00
206	ILE	CB	-34.33	-29.12	54.62	15.00
206	ILE	CG2	-35.41	-30.09	54.17	15.00
206	ILE	CG1	-34.60	-28.70	56.06	15.00
206	ILE	CD1	-35.73	-27.69	56.23	15.00
206	ILE	C	-32.75	-31.00	55.45	15.00
206	ILE	O	-32.59	-30.85	56.66	15.00

207	ALA	N	-32.81	-32.22	54.92	15.00
207	ALA	CA	-32.67	-33.38	55.79	15.00
207	ALA	CB	-33.80	-34.33	55.58	15.00
207	ALA	C	-31.34	-34.09	55.63	15.00
207	ALA	O	-31.17	-35.20	56.13	15.00
208	ASN	N	-30.36	-33.45	55.00	15.00
208	ASN	CA	-29.04	-34.07	54.76	15.00
208	ASN	CB	-28.34	-33.45	53.52	15.00
208	ASN	CG	-28.78	-34.07	52.18	15.00
208	ASN	OD1	-29.25	-35.21	52.11	15.00
208	ASN	ND2	-28.60	-33.31	51.12	15.00
208	ASN	C	-28.08	-34.01	55.94	15.00
208	ASN	O	-27.28	-34.93	56.15	15.00
209	LEU	N	-28.08	-32.88	56.64	15.00
209	LEU	CA	-27.19	-32.64	57.78	15.00
209	LEU	CB	-26.07	-31.64	57.40	15.00
209	LEU	CG	-24.73	-31.69	58.15	15.00
209	LEU	CD1	-24.11	-33.07	58.09	15.00
209	LEU	CD2	-23.76	-30.66	57.52	15.00
209	LEU	C	-27.97	-32.12	59.02	15.00
209	LEU	O	-27.72	-30.99	59.50	15.00
210	ALA	N	-28.79	-32.99	59.65	15.00
210	ALA	H	-29.19	-33.47	58.90	15.00
210	ALA	CA	-29.59	-32.51	60.77	15.00
210	ALA	CB	-31.08	-32.79	60.54	15.00
210	ALA	C	-29.19	-33.24	62.06	15.00
210	ALA	O	-28.91	-34.44	62.09	15.00
211	SER	N	-29.24	-32.48	63.17	15.00
211	SER	CA	-28.94	-33.06	64.47	15.00
211	SER	CB	-27.44	-33.22	64.70	15.00
211	SER	OG	-26.78	-31.96	64.75	15.00
211	SER	C	-29.57	-32.31	65.62	15.00
211	SER	O	-30.17	-31.24	65.41	15.00
212	PHE	N	-29.43	-32.92	66.81	15.00
212	PHE	CA	-29.96	-32.40	68.07	15.00
212	PHE	CB	-31.46	-32.75	68.27	15.00
212	PHE	CG	-31.78	-34.22	68.27	15.00
212	PHE	CD1	-32.33	-34.84	67.14	15.00
212	PHE	CD2	-31.61	-34.97	69.41	15.00
212	PHE	CE1	-32.71	-36.19	67.17	15.00
212	PHE	CE2	-31.98	-36.30	69.45	15.00
212	PHE	CZ	-32.54	-36.91	68.33	15.00
212	PHE	C	-29.16	-32.88	69.27	15.00

212 PHE O	-28.56	-33.95	69.23	15.00
213 PRO N	-29.11	-32.06	70.33	15.00
213 PRO CD	-29.69	-30.71	70.50	15.00
213 PRO CA	-28.36	-32.43	71.53	15.00
213 PRO CB	-28.14	-31.08	72.20	15.00
213 PRO CG	-29.45	-30.47	72.01	15.00
213 PRO C	-29.19	-33.38	72.46	15.00
213 PRO O	-30.42	-33.47	72.36	15.00
214 LYS N	-28.53	-34.16	73.30	15.00
214 LYS CA	-29.24	-35.05	74.22	15.00
214 LYS CB	-28.57	-36.43	74.20	15.00
214 LYS CG	-28.79	-37.24	72.91	15.00
214 LYS CD	-28.01	-38.56	72.92	15.00
214 LYS CE	-28.46	-39.53	71.81	15.00
214 LYS NZ	-27.39	-40.57	71.71	15.00
214 LYS C	-29.05	-34.34	75.56	15.00
214 LYS O	-27.98	-33.76	75.79	15.00
215 MET N	-30.08	-34.35	76.41	15.00
215 MET CA	-29.99	-33.65	77.70	15.00
215 MET CB	-31.12	-32.61	77.90	15.00
215 MET CG	-30.96	-31.28	77.20	15.00
215 MET SD	-29.93	-30.01	77.96	15.00
215 MET CE	-31.16	-28.81	78.53	15.00
215 MET C	-29.93	-34.56	78.90	15.00
215 MET OT1	-28.98	-34.44	79.69	15.00
215 MET OT2	-30.83	-35.40	79.08	15.00
216 HOH OH2	-32.26	-16.46	65.37	15.00
217 HOH OH2	-29.10	-19.91	62.23	15.00
218 HOH OH2	-10.46	-12.34	64.01	15.00
219 HOH OH2	-16.64	-12.04	73.86	15.00
220 HOH OH2	-35.65	-23.61	70.00	15.00
221 HOH OH2	-30.42	-35.41	58.75	15.00
222 HOH OH2	-31.55	-20.39	66.10	15.00
223 HOH OH2	-25.68	-31.53	62.01	15.00
224 HOH OH2	-12.63	-8.84	62.20	15.00
225 HOH OH2	-14.75	-22.14	66.35	15.00
226 HOH OH2	-44.50	-27.54	49.50	15.00
227 HOH OH2	-46.66	-35.25	56.37	15.00
228 HOH OH2	-41.69	-17.81	69.13	15.00
229 HOH OH2	-31.65	-20.57	63.48	15.00
230 HOH OH2	-19.45	-17.08	56.43	15.00
231 HOH OH2	-14.47	-31.20	62.15	15.00
232 HOH OH2	-44.49	-25.37	44.32	15.00

233	HOH	OH2	-23.11	-31.07	62.02	15.00
234	HOH	OH2	-24.80	-4.69	68.36	15.00
235	HOH	OH2	-31.22	-18.66	68.39	15.00
236	HOH	OH2	-37.21	-27.28	51.82	15.00
237	HOH	OH2	-37.54	-25.42	49.65	15.00
238	HOH	OH2	-48.22	-33.37	57.46	15.00
239	HOH	OH2	-29.06	-10.11	76.59	15.00
240	HOH	OH2	-35.53	-14.09	77.20	15.00
241	HOH	OH2	-16.66	-4.74	70.29	15.00
242	HOH	OH2	-17.42	-8.40	75.32	15.00
243	HOH	OH2	-10.92	-18.14	70.16	15.00
244	HOH	OH2	-9.58	-20.04	78.06	15.00
245	HOH	OH2	-46.35	-17.06	54.42	15.00
246	HOH	OH2	-34.19	-29.40	45.76	15.00
247	HOH	OH2	-36.78	-37.90	52.62	15.00
248	HOH	OH2	-42.43	-35.18	56.19	15.00
249	HOH	OH2	-41.62	-19.52	71.38	15.00
250	HOH	OH2	-48.81	-19.01	73.95	15.00
251	HOH	OH2	-41.55	-15.71	71.06	15.00
252	HOH	OH2	-26.21	-9.24	68.97	15.00
253	HOH	OH2	-33.78	-8.96	64.11	15.00
254	HOH	OH2	-20.04	-8.25	62.53	15.00
255	HOH	OH2	-17.20	-6.33	64.20	15.00
256	HOH	OH2	-35.58	-40.12	65.37	15.00
257	HOH	OH2	-13.46	-24.38	76.78	15.00
258	HOH	OH2	-8.00	-25.77	61.24	15.00
259	HOH	OH2	-21.06	-27.44	51.53	15.00
260	HOH	OH2	-25.94	-34.05	61.10	15.00
261	HOH	OH2	-12.35	-29.04	72.99	15.00
262	HOH	OH2	-33.29	-40.38	63.87	15.00
263	HOH	OH2	-20.24	-23.70	87.14	15.00
264	HOH	OH2	-13.21	-12.02	62.79	15.00
265	HOH	OH2	-21.34	-33.08	61.27	15.00
266	HOH	OH2	-29.60	-16.68	41.72	15.00
267	HOH	OH2	-25.80	-19.25	42.13	15.00
268	HOH	OH2	-32.98	-34.45	47.05	15.00
269	HOH	OH2	-23.16	-31.07	42.89	15.00
270	HOH	OH2	-34.03	-29.11	42.28	15.00
271	HOH	OH2	-36.71	-26.01	46.91	15.00

Table of the orthogonal three dimensional coordinates in
Ångstroms and B factors (\AA^2) for the cathepsin K
complex with inhibitor 4-[N-
[(phenylmethoxy)carbonyl]-L-leucyl]-1-N[N-(methyl)-
L-leucyl]]-3-pyrrolidinone.

Residue Atom	X	Y	Z	B
1 ALA CB	-54.23	-33.20	65.64	15.00
1 ALA C	-53.54	-33.00	63.24	15.00
1 ALA O	-52.73	-33.83	62.79	15.00
1 ALA N	-54.89	-34.90	63.97	15.00
1 ALA CA	-54.65	-33.45	64.19	15.00
2 PRO N	-53.49	-31.70	62.91	15.00
2 PRO CD	-54.26	-30.56	63.46	15.00
2 PRO CA	-52.44	-31.22	62.00	15.00
2 PRO CB	-52.58	-29.69	62.07	15.00
2 PRO CG	-53.25	-29.45	63.41	15.00
2 PRO C	-51.07	-31.68	62.50	15.00
2 PRO O	-50.74	-31.50	63.67	15.00
3 ASP N	-50.31	-32.35	61.64	15.00
3 ASP CA	-48.98	-32.84	62.01	15.00
3 ASP CB	-48.55	-33.98	61.08	15.00
3 ASP CG	-47.66	-35.01	61.77	15.00
3 ASP OD1	-46.52	-34.66	62.18	15.00
3 ASP OD2	-48.10	-36.17	61.89	15.00
3 ASP C	-48.00	-31.68	61.94	15.00
3 ASP O	-47.13	-31.65	61.06	15.00
4 SER N	-48.12	-30.72	62.85	15.00
4 SER CA	-47.23	-29.56	62.86	15.00
4 SER CB	-47.87	-28.37	62.15	15.00
4 SER OG	-49.05	-27.95	62.82	15.00
4 SER C	-46.76	-29.14	64.25	15.00
4 SER O	-47.54	-29.19	65.22	15.00
5 VAL N	-45.50	-28.70	64.35	15.00
5 VAL CA	-44.91	-28.26	65.61	15.00
5 VAL CB	-43.77	-29.21	66.10	15.00
5 VAL CG1	-43.35	-28.82	67.51	15.00
5 VAL CG2	-44.19	-30.65	66.04	15.00
5 VAL C	-44.29	-26.87	65.45	15.00
5 VAL O	-43.47	-26.65	64.55	15.00
6 ASP N	-44.64	-25.95	66.33	15.00

6 ASP CA	-44.10	-24.60	66.28	15.00
6 ASP CB	-45.17	-23.57	65.90	15.00
6 ASP CG	-44.59	-22.26	65.40	15.00
6 ASP OD1	-43.41	-21.95	65.68	15.00
6 ASP OD2	-45.34	-21.52	64.73	15.00
6 ASP C	-43.52	-24.32	67.66	15.00
6 ASP O	-44.20	-23.78	68.53	15.00
7 TYR N	-42.27	-24.69	67.85	15.00
7 TYR CA	-41.62	-24.50	69.13	15.00
7 TYR CB	-40.20	-25.08	69.12	15.00
7 TYR CG	-40.20	-26.58	69.20	15.00
7 TYR CD1	-40.68	-27.24	70.33	15.00
7 TYR CE1	-40.76	-28.62	70.38	15.00
7 TYR CD2	-39.81	-27.36	68.11	15.00
7 TYR CE2	-39.89	-28.74	68.15	15.00
7 TYR CZ	-40.37	-29.36	69.29	15.00
7 TYR OH	-40.51	-30.72	69.31	15.00
7 TYR C	-41.63	-23.07	69.62	15.00
7 TYR O	-41.57	-22.84	70.83	15.00
8 ARG N	-41.74	-22.11	68.70	15.00
8 ARG CA	-41.77	-20.68	69.08	15.00
8 ARG CB	-41.86	-19.77	67.84	15.00
8 ARG CG	-40.77	-19.98	66.80	15.00
8 ARG CD	-41.01	-19.12	65.58	15.00
8 ARG NE	-42.34	-19.33	65.02	15.00
8 ARG CZ	-42.70	-18.96	63.80	15.00
8 ARG NH1	-41.83	-18.36	63.00	15.00
8 ARG NH2	-43.94	-19.18	63.38	15.00
8 ARG C	-42.94	-20.39	70.02	15.00
8 ARG O	-42.79	-19.67	71.02	15.00
9 LYS N	-44.10	-20.98	69.72	15.00
9 LYS CA	-45.29	-20.80	70.53	15.00
9 LYS CB	-46.53	-21.26	69.78	15.00
9 LYS CG	-46.84	-20.43	68.56	15.00
9 LYS CD	-48.15	-20.86	67.92	15.00
9 LYS CE	-48.39	-20.11	66.62	15.00
9 LYS NZ	-49.58	-20.62	65.88	15.00
9 LYS C	-45.18	-21.53	71.85	15.00
9 LYS O	-45.95	-21.29	72.77	15.00
10 LYS N	-44.18	-22.40	71.95	15.00
10 LYS CA	-43.99	-23.17	73.16	15.00
10 LYS CB	-43.71	-24.63	72.80	15.00

10	LYS	CG	-44.67	-25.19	71.78	15.00
10	LYS	CD	-44.34	-26.64	71.49	15.00
10	LYS	CE	-44.42	-27.48	72.76	15.00
10	LYS	NZ	-45.74	-27.26	73.43	15.00
10	LYS	C	-42.92	-22.65	74.11	15.00
10	LYS	O	-42.70	-23.25	75.15	15.00
11	GLY	N	-42.24	-21.57	73.73	15.00
11	GLY	CA	-41.21	-21.00	74.58	15.00
11	GLY	C	-39.83	-21.65	74.47	15.00
11	GLY	O	-38.92	-21.31	75.21	15.00
12	TYR	N	-39.68	-22.56	73.52	15.00
12	TYR	CA	-38.41	-23.26	73.31	15.00
12	TYR	CB	-38.63	-24.56	72.54	15.00
12	TYR	CG	-39.27	-25.70	73.30	15.00
12	TYR	CD1	-40.37	-25.50	74.13	15.00
12	TYR	CE1	-40.97	-26.57	74.82	15.00
12	TYR	CD2	-38.78	-27.00	73.17	15.00
12	TYR	CE2	-39.37	-28.07	73.84	15.00
12	TYR	CZ	-40.45	-27.85	74.66	15.00
12	TYR	OH	-41.02	-28.91	75.33	15.00
12	TYR	C	-37.36	-22.43	72.56	15.00
12	TYR	O	-36.22	-22.86	72.46	15.00
13	VAL	N	-37.76	-21.27	72.03	15.00
13	VAL	CA	-36.86	-20.43	71.23	15.00
13	VAL	CB	-37.38	-20.33	69.78	15.00
13	VAL	CG1	-36.34	-19.72	68.89	15.00
13	VAL	CG2	-37.75	-21.69	69.26	15.00
13	VAL	C	-36.62	-19.00	71.75	15.00
13	VAL	O	-37.55	-18.32	72.18	15.00
14	THR	N	-35.38	-18.53	71.67	15.00
14	THR	CA	-35.04	-17.18	72.11	15.00
14	THR	CB	-33.58	-17.11	72.54	15.00
14	THR	OG1	-32.76	-17.76	71.55	15.00
14	THR	CG2	-33.39	-17.76	73.88	15.00
14	THR	C	-35.25	-16.15	70.99	15.00
14	THR	O	-35.59	-16.51	69.86	15.00
15	PRO	N	-35.10	-14.85	71.31	15.00
15	PRO	CD	-35.02	-14.21	72.63	15.00
15	PRO	CA	-35.29	-13.83	70.27	15.00
15	PRO	CB	-35.03	-12.54	71.03	15.00
15	PRO	CG	-35.58	-12.84	72.37	15.00
15	PRO	C	-34.27	-14.02	69.14	15.00

15	PRO O	-33.20	-14.57	69.36	15.00
16	VAL N	-34.63	-13.62	67.92	15.00
16	VAL CA	-33.72	-13.74	66.79	15.00
16	VAL CB	-34.41	-13.41	65.45	15.00
16	VAL CG1	-33.40	-13.43	64.31	15.00
16	VAL CG2	-35.52	-14.40	65.18	15.00
16	VAL C	-32.53	-12.82	67.01	15.00
16	VAL O	-32.69	-11.69	67.46	15.00
17	LYS N	-31.34	-13.30	66.69	15.00
17	LYS CA	-30.16	-12.50	66.88	15.00
17	LYS CB	-29.27	-13.11	67.95	15.00
17	LYS CG	-29.97	-13.18	69.30	15.00
17	LYS CD	-29.17	-13.95	70.33	15.00
17	LYS CE	-29.96	-14.12	71.61	15.00
17	LYS NZ	-31.23	-14.87	71.36	15.00
17	LYS C	-29.41	-12.30	65.58	15.00
17	LYS O	-29.51	-13.11	64.66	15.00
18	ASN N	-28.68	-11.18	65.51	15.00
18	ASN CA	-27.89	-10.84	64.33	15.00
18	ASN CB	-28.01	-9.37	63.99	15.00
18	ASN CG	-27.30	-9.03	62.72	15.00
18	ASN OD1	-27.10	-9.90	61.88	15.00
18	ASN ND2	-26.89	-7.78	62.57	15.00
18	ASN C	-26.42	-11.21	64.52	15.00
18	ASN O	-25.77	-10.70	65.43	15.00
19	GLN N	-25.89	-12.04	63.63	15.00
19	GLN CA	-24.50	-12.46	63.73	15.00
19	GLN CB	-24.24	-13.75	62.96	15.00
19	GLN CG	-24.32	-13.63	61.47	15.00
19	GLN CD	-24.07	-14.96	60.80	15.00
19	GLN OE1	-25.01	-15.66	60.43	15.00
19	GLN NE2	-22.81	-15.32	60.65	15.00
19	GLN C	-23.48	-11.40	63.36	15.00
19	GLN O	-22.32	-11.48	63.76	15.00
20	GLY N	-23.90	-10.40	62.59	15.00
20	GLY CA	-22.99	-9.33	62.22	15.00
20	GLY C	-21.93	-9.72	61.22	15.00
20	GLY O	-22.06	-10.71	60.52	15.00
21	GLN N	-20.86	-8.94	61.15	15.00
21	GLN CA	-19.79	-9.22	60.22	15.00
21	GLN CB	-19.10	-7.92	59.77	15.00
21	GLN CG	-20.08	-6.82	59.31	15.00

21 GLN CD	-21.21	-7.35	58.42	15.00
21 GLN OE1	-20.98	-7.83	57.31	15.00
21 GLN NE2	-22.44	-7.28	58.92	15.00
21 GLN C	-18.81	-10.21	60.83	15.00
21 GLN O	-17.67	-9.87	61.14	15.00
22 CYS N	-19.29	-11.45	61.00	15.00
22 CYS CA	-18.53	-12.54	61.60	15.00
22 CYS C	-19.20	-13.84	61.19	15.00
22 CYS O	-20.43	-13.93	61.23	15.00
22 CYS CB	-18.48	-12.40	63.13	15.00
22 CYS SG	-18.13	-13.92	64.07	15.00
23 GLY N	-18.42	-14.83	60.76	15.00
23 GLY CA	-19.01	-16.09	60.33	15.00
23 GLY C	-19.33	-17.04	61.47	15.00
23 GLY O	-18.80	-18.16	61.54	15.00
24 SER N	-20.21	-16.60	62.36	15.00
24 SER CA	-20.58	-17.40	63.52	15.00
24 SER CB	-20.34	-16.63	64.80	15.00
24 SER OG	-21.04	-15.40	64.76	15.00
24 SER C	-22.00	-17.93	63.45	15.00
24 SER O	-22.68	-18.02	64.46	15.00
25 CYS N	-22.46	-18.32	62.28	15.00
25 CYS CA	-23.80	-18.84	62.17	15.00
25 CYS CB	-24.25	-18.85	60.71	15.00
25 CYS SG	-23.19	-19.72	59.59	15.00
25 CYS C	-23.89	-20.22	62.84	15.00
25 CYS O	-24.95	-20.62	63.34	15.00
25 INH C1	-26.58	-9.77	58.47	15.00
25 INH C2	-26.25	-10.40	57.28	15.00
25 INH C3	-25.06	-11.13	57.18	15.00
25 INH C4	-24.20	-11.22	58.27	15.00
25 INH C5	-24.54	-10.58	59.46	15.00
25 INH C6	-25.72	-9.86	59.56	15.00
25 INH C7	-22.95	-12.04	58.18	15.00
25 INH O8	-22.93	-12.74	56.96	15.00
25 INH C9	-23.31	-14.09	56.78	15.00
25 INH O10	-24.36	-14.56	57.24	15.00
25 INH C11	-22.67	-16.23	55.81	15.00
25 INH C12	-22.36	-16.56	54.34	15.00
25 INH C13	-23.44	-17.20	53.45	15.00
25 INH C14	-24.11	-18.35	54.17	15.00
25 INH C15	-24.46	-16.19	52.94	15.00

25 INH C16	-21.76	-17.01	56.78	15.00
25 INH O17	-20.87	-16.42	57.43	15.00
25 INH N18	-21.99	-18.32	56.91	15.00
25 INH C19	-21.15	-18.98	57.84	15.00
25 INH N20	-22.45	-14.81	56.08	15.00
25 INH C21	-20.81	-20.41	57.54	15.00
25 INH C22	-21.63	-18.99	59.30	15.00
25 INH O23	-21.62	-17.88	59.81	15.00
25 INH C24	-17.90	-23.12	57.09	15.00
25 INH C25	-20.20	-23.31	57.89	15.00
25 INH C26	-21.15	-24.49	58.06	15.00
25 INH C27	-21.28	-25.45	56.87	15.00
25 INH C28	-19.93	-25.80	56.26	15.00
25 INH C29	-22.00	-26.71	57.30	15.00
25 INH C30	-20.37	-22.34	59.06	15.00
25 INH O31	-20.24	-22.76	60.20	15.00
25 INH N32	-20.66	-21.04	58.80	15.00
25 INH C33	-20.82	-20.11	59.89	15.00
25 INH N34	-18.81	-23.74	57.85	15.00
26 TRP N	-22.76	-20.93	62.89	15.00
26 TRP CA	-22.67	-22.24	63.53	15.00
26 TRP CB	-21.35	-22.95	63.19	15.00
26 TRP CG	-20.14	-22.22	63.67	15.00
26 TRP CD2	-19.45	-22.41	64.92	15.00
26 TRP CE2	-18.44	-21.43	65.00	15.00
26 TRP CE3	-19.61	-23.30	65.99	15.00
26 TRP CD1	-19.51	-21.18	63.05	15.00
26 TRP NE1	-18.50	-20.70	63.84	15.00
26 TRP CZ2	-17.59	-21.32	66.10	15.00
26 TRP CZ3	-18.76	-23.19	67.08	15.00
26 TRP CH2	-17.76	-22.21	67.13	15.00
26 TRP C	-22.83	-22.09	65.05	15.00
26 TRP O	-23.50	-22.90	65.69	15.00
27 ALA N	-22.22	-21.05	65.60	15.00
27 ALA CA	-22.28	-20.76	67.03	15.00
27 ALA CB	-21.34	-19.64	67.37	15.00
27 ALA C	-23.71	-20.40	67.41	15.00
27 ALA O	-24.15	-20.67	68.53	15.00
28 PHE N	-24.44	-19.79	66.48	15.00
28 PHE CA	-25.83	-19.42	66.72	15.00
28 PHE CB	-26.28	-18.29	65.81	15.00
28 PHE CG	-25.77	-16.95	66.24	15.00

28 PHE CD1	-24.53	-16.50	65.83	15.00
28 PHE CD2	-26.52	-16.16	67.11	15.00
28 PHE CE1	-24.03	-15.31	66.28	15.00
28 PHE CE2	-26.02	-14.96	67.56	15.00
28 PHE CZ	-24.78	-14.53	67.15	15.00
28 PHE C	-26.76	-20.62	66.63	15.00
28 PHE O	-27.71	-20.74	67.40	15.00
29 SER N	-26.51	-21.50	65.67	15.00
29 SER CA	-27.33	-22.69	65.53	15.00
29 SER CB	-26.88	-23.54	64.35	15.00
29 SER OG	-27.59	-24.76	64.31	15.00
29 SER C	-27.22	-23.49	66.82	15.00
29 SER O	-28.20	-23.61	67.54	15.00
30 SER N	-26.01	-23.95	67.12	15.00
30 SER CA	-25.70	-24.75	68.32	15.00
30 SER CB	-24.19	-24.86	68.50	15.00
30 SER OG	-23.53	-25.04	67.27	15.00
30 SER C	-26.34	-24.24	69.61	15.00
30 SER O	-26.97	-25.00	70.37	15.00
31 VAL N	-26.15	-22.96	69.88	15.00
31 VAL CA	-26.71	-22.32	71.06	15.00
31 VAL CB	-26.23	-20.85	71.13	15.00
31 VAL CG1	-27.15	-20.01	71.98	15.00
31 VAL CG2	-24.83	-20.81	71.69	15.00
31 VAL C	-28.23	-22.44	71.03	15.00
31 VAL O	-28.86	-22.74	72.04	15.00
32 GLY N	-28.82	-22.26	69.85	15.00
32 GLY CA	-30.26	-22.36	69.72	15.00
32 GLY C	-30.78	-23.75	70.03	15.00
32 GLY O	-31.86	-23.89	70.62	15.00
33 ALA N	-30.07	-24.78	69.61	15.00
33 ALA CA	-30.50	-26.14	69.90	15.00
33 ALA CB	-29.65	-27.14	69.16	15.00
33 ALA C	-30.37	-26.36	71.40	15.00
33 ALA O	-31.29	-26.85	72.05	15.00
34 LEU N	-29.24	-25.92	71.96	15.00
34 LEU CA	-28.96	-26.04	73.40	15.00
34 LEU CB	-27.57	-25.50	73.75	15.00
34 LEU CG	-26.28	-26.23	73.40	15.00
34 LEU CD1	-25.11	-25.32	73.73	15.00
34 LEU CD2	-26.17	-27.53	74.19	15.00
34 LEU C	-30.00	-25.35	74.28	15.00

34 LEU O	-30.28	-25.81	75.38	15.00
35 GLU N	-30.49	-24.21	73.82	15.00
35 GLU CA	-31.50	-23.44	74.55	15.00
35 GLU CB	-31.65	-22.02	74.01	15.00
35 GLU CG	-30.41	-21.16	74.08	15.00
35 GLU CD	-30.48	-19.98	73.14	15.00
35 GLU OE1	-31.23	-20.04	72.14	15.00
35 GLU OE2	-29.79	-18.98	73.39	15.00
35 GLU C	-32.84	-24.14	74.47	15.00
35 GLU O	-33.60	-24.12	75.44	15.00
36 GLY N	-33.13	-24.71	73.31	15.00
36 GLY CA	-34.38	-25.43	73.12	15.00
36 GLY C	-34.45	-26.58	74.11	15.00
36 GLY O	-35.47	-26.75	74.79	15.00
37 GLN N	-33.35	-27.32	74.22	15.00
37 GLN CA	-33.25	-28.43	75.15	15.00
37 GLN CB	-32.05	-29.31	74.83	15.00
37 GLN CG	-32.27	-30.21	73.64	15.00
37 GLN CD	-33.50	-31.08	73.81	15.00
37 GLN OE1	-33.74	-31.63	74.88	15.00
37 GLN NE2	-34.28	-31.20	72.75	15.00
37 GLN C	-33.22	-27.96	76.60	15.00
37 GLN O	-33.78	-28.61	77.48	15.00
38 LEU N	-32.60	-26.81	76.84	15.00
38 LEU CA	-32.52	-26.23	78.19	15.00
38 LEU CB	-31.72	-24.94	78.20	15.00
38 LEU CG	-31.57	-24.25	79.55	15.00
38 LEU CD1	-30.61	-25.04	80.42	15.00
38 LEU CD2	-31.08	-22.82	79.38	15.00
38 LEU C	-33.94	-26.00	78.70	15.00
38 LEU O	-34.27	-26.33	79.83	15.00
39 LYS N	-34.78	-25.42	77.86	15.00
39 LYS CA	-36.17	-25.16	78.19	15.00
39 LYS CB	-36.85	-24.36	77.08	15.00
39 LYS CG	-38.38	-24.43	77.06	15.00
39 LYS CD	-39.03	-23.68	78.21	15.00
39 LYS CE	-40.52	-23.93	78.24	15.00
39 LYS NZ	-41.17	-23.27	79.40	15.00
39 LYS C	-36.89	-26.48	78.42	15.00
39 LYS O	-37.73	-26.59	79.30	15.00
40 LYS N	-36.56	-27.49	77.63	15.00
40 LYS CA	-37.20	-28.78	77.78	15.00

40 LYS CB	-36.83	-29.73	76.64	15.00
40 LYS CG	-37.74	-30.93	76.59	15.00
40 LYS CD	-37.39	-31.91	75.51	15.00
40 LYS CE	-38.47	-32.98	75.42	15.00
40 LYS NZ	-38.17	-34.02	74.40	15.00
40 LYS C	-36.89	-29.42	79.13	15.00
40 LYS O	-37.79	-29.93	79.80	15.00
41 LYS N	-35.62	-29.36	79.53	15.00
41 LYS CA	-35.17	-29.95	80.79	15.00
41 LYS CB	-33.65	-30.16	80.81	15.00
41 LYS CG	-33.08	-30.87	79.59	15.00
41 LYS CD	-33.91	-32.09	79.21	15.00
41 LYS CE	-33.34	-32.77	77.99	15.00
41 LYS NZ	-34.29	-33.81	77.44	15.00
41 LYS C	-35.59	-29.16	82.02	15.00
41 LYS O	-36.42	-29.61	82.81	15.00
42 THR N	-35.01	-27.98	82.17	15.00
42 THR CA	-35.26	-27.11	83.32	15.00
42 THR CB	-34.10	-26.13	83.49	15.00
42 THR OG1	-34.11	-25.20	82.40	15.00
42 THR CG2	-32.77	-26.87	83.51	15.00
42 THR C	-36.58	-26.34	83.35	15.00
42 THR O	-36.92	-25.75	84.37	15.00
43 GLY N	-37.30	-26.30	82.24	15.00
43 GLY CA	-38.56	-25.58	82.19	15.00
43 GLY C	-38.44	-24.08	82.03	15.00
43 GLY O	-39.45	-23.39	81.86	15.00
44 LYS N	-37.22	-23.56	82.10	15.00
44 LYS CA	-36.96	-22.13	81.97	15.00
44 LYS CB	-36.42	-21.56	83.28	15.00
44 LYS CG	-37.47	-21.47	84.38	15.00
44 LYS CD	-36.85	-21.18	85.72	15.00
44 LYS CE	-36.08	-22.36	86.23	15.00
44 LYS NZ	-37.00	-23.52	86.37	15.00
44 LYS C	-35.99	-21.90	80.82	15.00
44 LYS O	-35.12	-22.73	80.57	15.00
45 LEU N	-36.16	-20.79	80.10	15.00
45 LEU CA	-35.31	-20.46	78.95	15.00
45 LEU CB	-36.19	-20.14	77.73	15.00
45 LEU CG	-35.60	-19.92	76.34	15.00
45 LEU CD1	-35.30	-21.23	75.64	15.00
45 LEU CD2	-36.62	-19.13	75.55	15.00

45 LEU C	-34.32	-19.32	79.23	15.00
45 LEU O	-34.65	-18.34	79.89	15.00
46 LEU N	-33.11	-19.46	78.68	15.00
46 LEU CA	-32.02	-18.47	78.83	15.00
46 LEU CB	-30.97	-18.94	79.82	15.00
46 LEU CG	-30.95	-18.53	81.29	15.00
46 LEU CD1	-29.80	-19.23	81.98	15.00
46 LEU CD2	-30.80	-17.02	81.38	15.00
46 LEU C	-31.33	-18.24	77.48	15.00
46 LEU O	-31.36	-19.10	76.62	15.00
47 ASN N	-30.68	-17.09	77.32	15.00
47 ASN CA	-29.95	-16.81	76.10	15.00
47 ASN CB	-29.88	-15.32	75.78	15.00
47 ASN CG	-31.23	-14.72	75.46	15.00
47 ASN OD1	-31.79	-13.96	76.25	15.00
47 ASN ND2	-31.74	-15.03	74.28	15.00
47 ASN C	-28.56	-17.33	76.35	15.00
47 ASN O	-27.87	-16.81	77.23	15.00
48 LEU N	-28.16	-18.41	75.67	15.00
48 LEU CA	-26.81	-18.95	75.85	15.00
48 LEU CB	-26.75	-20.44	75.51	15.00
48 LEU CG	-27.61	-21.41	76.33	15.00
48 LEU CD1	-27.10	-22.82	76.11	15.00
48 LEU CD2	-27.55	-21.06	77.80	15.00
48 LEU C	-25.82	-18.14	75.02	15.00
48 LEU O	-26.22	-17.32	74.19	15.00
49 SER N	-24.53	-18.38	75.23	15.00
49 SER CA	-23.48	-17.62	74.55	15.00
49 SER CB	-22.43	-17.16	75.56	15.00
49 SER OG	-21.36	-16.51	74.91	15.00
49 SER C	-22.77	-18.19	73.33	15.00
49 SER O	-21.87	-19.03	73.46	15.00
50 PRO N	-23.11	-17.69	72.12	15.00
50 PRO CD	-24.26	-16.83	71.79	15.00
50 PRO CA	-22.46	-18.17	70.90	15.00
50 PRO CB	-23.32	-17.56	69.80	15.00
50 PRO CG	-23.89	-16.34	70.43	15.00
50 PRO C	-21.01	-17.66	70.85	15.00
50 PRO O	-20.16	-18.22	70.16	15.00
51 GLN N	-20.74	-16.59	71.61	15.00
51 GLN CA	-19.41	-15.98	71.71	15.00
51 GLN CB	-19.50	-14.57	72.29	15.00

51 GLN CG	-18.18	-13.80	72.34	15.00
51 GLN CD	-17.66	-13.43	70.96	15.00
51 GLN OE1	-18.33	-12.73	70.19	15.00
51 GLN NE2	-16.45	-13.88	70.65	15.00
51 GLN C	-18.50	-16.86	72.56	15.00
51 GLN O	-17.27	-16.82	72.42	15.00
52 ASN N	-19.11	-17.64	73.44	15.00
52 ASN CA	-18.38	-18.58	74.30	15.00
52 ASN CB	-19.35	-19.26	75.26	15.00
52 ASN CG	-18.67	-20.14	76.30	15.00
52 ASN OD1	-18.91	-19.99	77.51	15.00
52 ASN ND2	-17.88	-21.11	75.85	15.00
52 ASN C	-17.74	-19.57	73.32	15.00
52 ASN O	-16.55	-19.90	73.41	15.00
53 LEU N	-18.55	-20.00	72.36	15.00
53 LEU CA	-18.11	-20.96	71.35	15.00
53 LEU CB	-19.32	-21.52	70.61	15.00
53 LEU CG	-20.38	-22.09	71.55	15.00
53 LEU CD1	-21.65	-22.44	70.79	15.00
53 LEU CD2	-19.83	-23.30	72.25	15.00
53 LEU C	-17.06	-20.37	70.39	15.00
53 LEU O	-15.94	-20.89	70.28	15.00
54 VAL N	-17.43	-19.27	69.73	15.00
54 VAL CA	-16.55	-18.58	68.78	15.00
54 VAL CB	-17.06	-17.14	68.52	15.00
54 VAL CG1	-16.12	-16.40	67.60	15.00
54 VAL CG2	-18.46	-17.18	67.91	15.00
54 VAL C	-15.12	-18.49	69.29	15.00
54 VAL O	-14.16	-18.68	68.55	15.00
55 ASP N	-15.00	-18.21	70.58	15.00
55 ASP CA	-13.71	-18.08	71.23	15.00
55 ASP CB	-13.82	-17.19	72.49	15.00
55 ASP CG	-14.16	-15.76	72.16	15.00
55 ASP OD1	-13.98	-15.35	71.00	15.00
55 ASP OD2	-14.62	-15.03	73.06	15.00
55 ASP C	-13.05	-19.41	71.60	15.00
55 ASP O	-11.98	-19.76	71.08	15.00
56 CYS N	-13.74	-20.18	72.43	15.00
56 CYS CA	-13.21	-21.42	72.96	15.00
56 CYS C	-13.19	-22.70	72.14	15.00
56 CYS O	-12.40	-23.59	72.45	15.00
56 CYS CB	-13.84	-21.68	74.32	15.00

56	CYS	SG	-14.09	-20.14	75.26	15.00
57	VAL	N	-14.06	-22.83	71.15	15.00
57	VAL	CA	-14.11	-24.04	70.33	15.00
57	VAL	CB	-15.47	-24.21	69.61	15.00
57	VAL	CG1	-15.58	-25.61	69.01	15.00
57	VAL	CG2	-16.61	-23.97	70.58	15.00
57	VAL	C	-12.98	-24.06	69.30	15.00
57	VAL	O	-13.18	-23.78	68.12	15.00
58	SER	N	-11.80	-24.45	69.76	15.00
58	SER	CA	-10.60	-24.55	68.94	15.00
58	SER	CB	-9.45	-25.07	69.79	15.00
58	SER	OG	-9.53	-24.53	71.10	15.00
58	SER	C	-10.73	-25.37	67.67	15.00
58	SER	O	-9.99	-25.17	66.72	15.00
59	GLU	N	-11.61	-26.36	67.70	15.00
59	GLU	CA	-11.83	-27.23	66.55	15.00
59	GLU	CB	-12.73	-28.41	66.92	15.00
59	GLU	CG	-12.20	-29.30	68.03	15.00
59	GLU	CD	-12.38	-28.71	69.41	15.00
59	GLU	OE1	-13.54	-28.51	69.82	15.00
59	GLU	OE2	-11.37	-28.43	70.06	15.00
59	GLU	C	-12.41	-26.48	65.37	15.00
59	GLU	O	-12.37	-26.95	64.23	15.00
60	ASN	N	-13.03	-25.34	65.65	15.00
60	ASN	CA	-13.65	-24.52	64.62	15.00
60	ASN	CB	-15.10	-24.18	64.99	15.00
60	ASN	CG	-16.04	-25.37	64.87	15.00
60	ASN	OD1	-17.24	-25.24	65.03	15.00
60	ASN	ND2	-15.49	-26.53	64.55	15.00
60	ASN	C	-12.83	-23.26	64.38	15.00
60	ASN	O	-11.82	-23.03	65.05	15.00
61	ASP	N	-13.28	-22.43	63.44	15.00
61	ASP	CA	-12.56	-21.22	63.09	15.00
61	ASP	CB	-12.53	-21.05	61.57	15.00
61	ASP	CG	-11.12	-20.82	61.03	15.00
61	ASP	OD1	-10.18	-20.65	61.83	15.00
61	ASP	OD2	-10.96	-20.82	59.79	15.00
61	ASP	C	-13.09	-19.95	63.76	15.00
61	ASP	O	-12.67	-18.85	63.43	15.00
62	GLY	N	-14.00	-20.09	64.72	15.00
62	GLY	CA	-14.55	-18.91	65.36	15.00
62	GLY	C	-15.40	-18.19	64.33	15.00

62 GLY O	-16.39	-18.75	63.85	15.00
63 CYS N	-14.98	-16.99	63.94	15.00
63 CYS CA	-15.70	-16.19	62.94	15.00
63 CYS C	-15.40	-16.66	61.53	15.00
63 CYS O	-15.88	-16.07	60.57	15.00
63 CYS CB	-15.39	-14.70	63.02	15.00
63 CYS SG	-16.14	-13.86	64.44	15.00
64 GLY N	-14.57	-17.68	61.40	15.00
64 GLY CA	-14.26	-18.20	60.08	15.00
64 GLY C	-15.21	-19.31	59.69	15.00
64 GLY O	-15.23	-19.74	58.53	15.00
65 GLY N	-15.99	-19.80	60.65	15.00
65 GLY CA	-16.93	-20.87	60.37	15.00
65 GLY C	-16.62	-22.14	61.14	15.00
65 GLY O	-15.48	-22.38	61.54	15.00
66 GLY N	-17.64	-22.95	61.35	15.00
66 GLY CA	-17.45	-24.19	62.08	15.00
66 GLY C	-18.56	-25.20	61.92	15.00
66 GLY O	-19.38	-25.12	61.00	15.00
67 TYR N	-18.56	-26.18	62.81	15.00
67 TYR CA	-19.55	-27.25	62.80	15.00
67 TYR CB	-18.89	-28.59	62.62	15.00
67 TYR CG	-18.09	-28.77	61.37	15.00
67 TYR CD1	-18.68	-28.65	60.11	15.00
67 TYR CE1	-17.97	-28.95	58.95	15.00
67 TYR CD2	-16.77	-29.18	61.44	15.00
67 TYR CE2	-16.05	-29.48	60.30	15.00
67 TYR CZ	-16.65	-29.37	59.06	15.00
67 TYR OH	-15.93	-29.71	57.94	15.00
67 TYR C	-20.31	-27.25	64.11	15.00
67 TYR O	-19.73	-26.97	65.15	15.00
68 MET N	-21.60	-27.57	64.06	15.00
68 MET CA	-22.40	-27.64	65.27	15.00
68 MET CB	-23.88	-27.79	64.94	15.00
68 MET CG	-24.47	-26.62	64.20	15.00
68 MET SD	-23.93	-26.55	62.51	15.00
68 MET CE	-25.32	-27.25	61.69	15.00
68 MET C	-21.91	-28.78	66.17	15.00
68 MET O	-21.81	-28.64	67.39	15.00
69 THR N	-21.56	-29.90	65.54	15.00
69 THR CA	-21.07	-31.07	66.27	15.00
69 THR CB	-20.66	-32.20	65.31	15.00

69 THR OG1	-19.57	-31.77	64.48	15.00
69 THR CG2	-21.84	-32.58	64.45	15.00
69 THR C	-19.91	-30.70	67.18	15.00
69 THR O	-19.94	-31.00	68.37	15.00
70 ASN N	-18.92	-30.00	66.64	15.00
70 ASN CA	-17.77	-29.54	67.42	15.00
70 ASN CB	-16.75	-28.84	66.55	15.00
70 ASN CG	-15.86	-29.80	65.85	15.00
70 ASN OD1	-15.33	-30.72	66.46	15.00
70 ASN ND2	-15.68	-29.61	64.55	15.00
70 ASN C	-18.17	-28.63	68.60	15.00
70 ASN O	-17.53	-28.66	69.66	15.00
71 ALA N	-19.20	-27.82	68.40	15.00
71 ALA CA	-19.67	-26.91	69.44	15.00
71 ALA CB	-20.66	-25.91	68.86	15.00
71 ALA C	-20.33	-27.72	70.55	15.00
71 ALA O	-20.26	-27.37	71.72	15.00
72 PHE N	-20.96	-28.83	70.16	15.00
72 PHE CA	-21.61	-29.70	71.13	15.00
72 PHE CB	-22.57	-30.66	70.43	15.00
72 PHE CG	-23.73	-29.98	69.79	15.00
72 PHE CD1	-24.28	-28.84	70.36	15.00
72 PHE CD2	-24.29	-30.48	68.63	15.00
72 PHE CE1	-25.35	-28.21	69.79	15.00
72 PHE CE2	-25.37	-29.87	68.04	15.00
72 PHE CZ	-25.91	-28.72	68.62	15.00
72 PHE C	-20.59	-30.46	71.96	15.00
72 PHE O	-20.79	-30.69	73.15	15.00
73 GLN N	-19.48	-30.82	71.33	15.00
73 GLN CA	-18.43	-31.54	72.03	15.00
73 GLN CB	-17.46	-32.17	71.04	15.00
73 GLN CG	-16.71	-33.36	71.59	15.00
73 GLN CD	-16.83	-34.56	70.67	15.00
73 GLN OE1	-17.35	-35.61	71.07	15.00
73 GLN NE2	-16.37	-34.41	69.44	15.00
73 GLN C	-17.70	-30.62	72.99	15.00
73 GLN O	-17.18	-31.07	74.02	15.00
74 TYR N	-17.64	-29.34	72.65	15.00
74 TYR CA	-16.96	-28.38	73.52	15.00
74 TYR CB	-16.74	-27.03	72.81	15.00
74 TYR CG	-16.38	-25.93	73.78	15.00
74 TYR CD1	-15.16	-25.95	74.45	15.00

74 TYR CE1	-14.87	-25.02	75.40	15.00
74 TYR CD2	-17.30	-24.94	74.11	15.00
74 TYR CE2	-17.01	-24.00	75.07	15.00
74 TYR CZ	-15.79	-24.05	75.71	15.00
74 TYR OH	-15.47	-23.11	76.67	15.00
74 TYR C	-17.69	-28.17	74.84	15.00
74 TYR O	-17.07	-28.14	75.89	15.00
75 VAL N	-19.00	-27.98	74.77	15.00
75 VAL CA	-19.82	-27.78	75.97	15.00
75 VAL CB	-21.29	-27.47	75.58	15.00
75 VAL CG1	-22.13	-27.23	76.82	15.00
75 VAL CG2	-21.34	-26.25	74.67	15.00
75 VAL C	-19.73	-29.01	76.87	15.00
75 VAL O	-19.82	-28.91	78.10	15.00
76 GLN N	-19.47	-30.16	76.26	15.00
76 GLN CA	-19.33	-31.42	76.97	15.00
76 GLN CB	-19.57	-32.58	76.01	15.00
76 GLN CG	-19.54	-33.95	76.62	15.00
76 GLN CD	-19.67	-35.03	75.58	15.00
76 GLN OE1	-20.73	-35.62	75.41	15.00
76 GLN NE2	-18.60	-35.28	74.86	15.00
76 GLN C	-17.96	-31.55	77.68	15.00
76 GLN O	-17.91	-31.76	78.89	15.00
77 LYS N	-16.87	-31.41	76.94	15.00
77 LYS CA	-15.53	-31.51	77.53	15.00
77 LYS CB	-14.43	-31.56	76.46	15.00
77 LYS CG	-14.07	-30.18	75.87	15.00
77 LYS CD	-12.80	-30.21	75.01	15.00
77 LYS CE	-13.01	-30.90	73.67	15.00
77 LYS NZ	-14.16	-30.32	72.90	15.00
77 LYS C	-15.26	-30.36	78.49	15.00
77 LYS O	-14.45	-30.49	79.41	15.00
78 ASN N	-15.89	-29.22	78.22	15.00
78 ASN CA	-15.73	-28.04	79.05	15.00
78 ASN CB	-16.05	-26.77	78.27	15.00
78 ASN CG	-15.64	-25.51	79.00	15.00
78 ASN OD1	-14.49	-25.35	79.40	15.00
78 ASN ND2	-16.57	-24.59	79.14	15.00
78 ASN C	-16.64	-28.15	80.26	15.00
78 ASN O	-16.46	-27.45	81.25	15.00
79 ARG N	-17.63	-29.04	80.16	15.00
79 ARG CA	-18.61	-29.26	81.22	15.00

79 ARG CB	-17.95	-29.71	82.54	15.00
79 ARG CG	-17.19	-31.05	82.52	15.00
79 ARG CD	-18.12	-32.28	82.55	15.00
79 ARG NE	-18.94	-32.34	83.76	15.00
79 ARG CZ	-20.14	-32.92	83.84	15.00
79 ARG NH1	-20.69	-33.51	82.78	15.00
79 ARG NH2	-20.82	-32.88	84.99	15.00
79 ARG C	-19.47	-28.02	81.44	15.00
79 ARG O	-19.86	-27.74	82.57	15.00
80 GLY N	-19.75	-27.27	80.38	15.00
80 GLY CA	-20.58	-26.08	80.52	15.00
80 GLY C	-20.38	-24.97	79.49	15.00
80 GLY O	-19.36	-24.93	78.78	15.00
81 ILE N	-21.37	-24.08	79.41	15.00
81 ILE CA	-21.35	-22.92	78.50	15.00
81 ILE CB	-22.14	-23.20	77.17	15.00
81 ILE CG2	-23.59	-23.57	77.46	15.00
81 ILE CG1	-22.11	-21.97	76.25	15.00
81 ILE CD1	-22.75	-22.19	74.90	15.00
81 ILE C	-22.00	-21.76	79.25	15.00
81 ILE O	-22.86	-21.98	80.11	15.00
82 ASP N	-21.56	-20.54	78.96	15.00
82 ASP CA	-22.09	-19.34	79.61	15.00
82 ASP CB	-21.08	-18.20	79.59	15.00
82 ASP CG	-19.89	-18.44	80.48	15.00
82 ASP OD1	-18.82	-17.87	80.21	15.00
82 ASP OD2	-20.03	-19.18	81.47	15.00
82 ASP C	-23.40	-18.85	79.02	15.00
82 ASP O	-23.89	-19.36	78.02	15.00
83 SER N	-23.96	-17.84	79.68	15.00
83 SER CA	-25.19	-17.20	79.27	15.00
83 SER CB	-26.03	-16.83	80.49	15.00
83 SER OG	-25.19	-16.35	81.52	15.00
83 SER C	-24.76	-15.96	78.49	15.00
83 SER O	-23.59	-15.58	78.53	15.00
84 GLU N	-25.68	-15.29	77.81	15.00
84 GLU CA	-25.29	-14.13	77.03	15.00
84 GLU CB	-26.39	-13.59	76.13	15.00
84 GLU CG	-25.83	-12.69	75.03	15.00
84 GLU CD	-24.85	-13.42	74.11	15.00
84 GLU OE1	-25.26	-13.79	72.99	15.00
84 GLU OE2	-23.68	-13.64	74.49	15.00

84	GLU C	-24.73	-13.05	77.92	15.00
84	GLU O	-23.52	-12.84	77.90	15.00
85	ASP N	-25.56	-12.36	78.69	15.00
85	ASP CA	-25.00	-11.32	79.55	15.00
85	ASP CB	-26.06	-10.32	80.06	15.00
85	ASP CG	-25.45	-8.93	80.42	15.00
85	ASP OD1	-26.14	-8.14	81.10	15.00
85	ASP OD2	-24.30	-8.62	80.02	15.00
85	ASP C	-24.32	-12.06	80.68	15.00
85	ASP O	-24.91	-12.29	81.73	15.00
86	ALA N	-23.11	-12.51	80.37	15.00
86	ALA CA	-22.20	-13.27	81.22	15.00
86	ALA CB	-22.80	-14.62	81.60	15.00
86	ALA C	-20.96	-13.46	80.33	15.00
86	ALA O	-19.83	-13.52	80.81	15.00
87	TYR N	-21.21	-13.59	79.03	15.00
87	TYR CA	-20.18	-13.73	78.00	15.00
87	TYR CB	-19.74	-15.19	77.86	15.00
87	TYR CG	-18.39	-15.40	77.19	15.00
87	TYR CD1	-17.78	-14.38	76.45	15.00
87	TYR CE1	-16.54	-14.59	75.84	15.00
87	TYR CD2	-17.73	-16.61	77.31	15.00
87	TYR CE2	-16.49	-16.82	76.72	15.00
87	TYR CZ	-15.90	-15.80	75.98	15.00
87	TYR OH	-14.67	-15.99	75.42	15.00
87	TYR C	-20.88	-13.21	76.73	15.00
87	TYR O	-21.25	-13.98	75.86	15.00
88	PRO N	-21.07	-11.89	76.64	15.00
88	PRO CD	-20.61	-10.92	77.65	15.00
88	PRO CA	-21.72	-11.18	75.54	15.00
88	PRO CB	-21.69	-9.73	76.00	15.00
88	PRO CG	-21.61	-9.83	77.49	15.00
88	PRO C	-21.11	-11.32	74.15	15.00
88	PRO O	-19.90	-11.51	74.00	15.00
89	TYR N	-21.95	-11.12	73.14	15.00
89	TYR CA	-21.55	-11.21	71.74	15.00
89	TYR CB	-22.75	-11.61	70.87	15.00
89	TYR CG	-22.36	-12.04	69.48	15.00
89	TYR CD1	-21.49	-13.11	69.29	15.00
89	TYR CE1	-21.07	-13.47	68.02	15.00
89	TYR CD2	-22.82	-11.36	68.36	15.00
89	TYR CE2	-22.41	-11.72	67.10	15.00

89 TYR CZ	-21.53	-12.77	66.94	15.00
89 TYR OH	-21.09	-13.11	65.69	15.00
89 TYR C	-20.90	-9.91	71.24	15.00
89 TYR O	-21.59	-8.91	71.03	15.00
90 VAL N	-19.58	-9.92	71.08	15.00
90 VAL CA	-18.87	-8.73	70.61	15.00
90 VAL CB	-17.41	-8.68	71.09	15.00
90 VAL CG1	-17.35	-8.79	72.60	15.00
90 VAL CG2	-16.59	-9.77	70.43	15.00
90 VAL C	-18.89	-8.68	69.08	15.00
90 VAL O	-18.82	-7.61	68.49	15.00
91 GLY N	-18.98	-9.84	68.45	15.00
91 GLY CA	-19.04	-9.87	67.01	15.00
91 GLY C	-17.71	-10.16	66.36	15.00
91 GLY O	-17.56	-9.93	65.16	15.00
92 GLN N	-16.76	-10.69	67.13	15.00
92 GLN CA	-15.43	-11.01	66.62	15.00
92 GLN CB	-14.62	-9.75	66.38	15.00
92 GLN CG	-14.24	-9.09	67.68	15.00
92 GLN CD	-13.83	-7.66	67.52	15.00
92 GLN OE1	-12.91	-7.19	68.19	15.00
92 GLN NE2	-14.53	-6.93	66.64	15.00
92 GLN C	-14.67	-11.92	67.58	15.00
92 GLN O	-14.91	-11.91	68.79	15.00
93 GLU N	-13.72	-12.66	67.02	15.00
93 GLU CA	-12.89	-13.59	67.78	15.00
93 GLU CB	-11.95	-14.35	66.85	15.00
93 GLU CG	-12.64	-15.06	65.69	15.00
93 GLU CD	-11.68	-15.45	64.57	15.00
93 GLU OE1	-10.56	-15.94	64.87	15.00
93 GLU OE2	-12.03	-15.24	63.39	15.00
93 GLU C	-12.11	-12.86	68.86	15.00
93 GLU O	-11.54	-11.79	68.61	15.00
94 GLU N	-12.08	-13.46	70.05	15.00
94 GLU CA	-11.38	-12.93	71.22	15.00
94 GLU CB	-12.31	-12.19	72.16	15.00
94 GLU CG	-12.77	-10.82	71.71	15.00
94 GLU CD	-13.69	-10.18	72.74	15.00
94 GLU OE1	-13.59	-8.95	72.97	15.00
94 GLU OE2	-14.50	-10.92	73.33	15.00
94 GLU C	-10.77	-14.12	71.96	15.00
94 GLU O	-11.15	-15.26	71.71	15.00

95 SER N	-9.87	-13.85	72.90	15.00
95 SER CA	-9.24	-14.91	73.69	15.00
95 SER CB	-8.09	-14.36	74.52	15.00
95 SER OG	-8.52	-13.24	75.28	15.00
95 SER C	-10.32	-15.52	74.59	15.00
95 SER O	-11.03	-14.78	75.28	15.00
96 CYS N	-10.42	-16.84	74.58	15.00
96 CYS CA	-11.43	-17.54	75.38	15.00
96 CYS C	-11.55	-17.08	76.82	15.00
96 CYS O	-10.69	-17.37	77.66	15.00
96 CYS CB	-11.24	-19.06	75.31	15.00
96 CYS SG	-12.40	-19.98	76.37	15.00
97 MET N	-12.60	-16.32	77.10	15.00
97 MET CA	-12.86	-15.80	78.44	15.00
97 MET CB	-13.16	-14.29	78.41	15.00
97 MET CG	-11.97	-13.37	78.13	15.00
97 MET SD	-12.05	-12.55	76.50	15.00
97 MET CE	-13.66	-11.72	76.66	15.00
97 MET C	-13.99	-16.57	79.13	15.00
97 MET O	-14.93	-15.96	79.66	15.00
98 TYR N	-13.91	-17.90	79.15	15.00
98 TYR CA	-14.96	-18.68	79.80	15.00
98 TYR CB	-14.79	-20.17	79.54	15.00
98 TYR CG	-15.85	-21.01	80.24	15.00
98 TYR CD1	-17.20	-20.84	79.95	15.00
98 TYR CE1	-18.17	-21.59	80.59	15.00
98 TYR CD2	-15.50	-21.96	81.19	15.00
98 TYR CE2	-16.48	-22.73	81.83	15.00
98 TYR CZ	-17.80	-22.53	81.53	15.00
98 TYR OH	-18.77	-23.27	82.16	15.00
98 TYR C	-15.11	-18.42	81.29	15.00
98 TYR O	-14.28	-18.80	82.11	15.00
99 ASN N	-16.21	-17.74	81.62	15.00
99 ASN CA	-16.59	-17.38	82.98	15.00
99 ASN CB	-17.52	-16.16	82.93	15.00
99 ASN CG	-17.93	-15.66	84.29	15.00
99 ASN OD1	-17.61	-16.27	85.32	15.00
99 ASN ND2	-18.65	-14.53	84.32	15.00
99 ASN C	-17.30	-18.62	83.57	15.00
99 ASN O	-18.50	-18.81	83.35	15.00
100 PRO N	-16.59	-19.46	84.35	15.00
100 PRO CD	-15.20	-19.31	84.81	15.00

100	PRO	CA	-17.20	-20.67	84.94	15.00
100	PRO	CB	-16.06	-21.26	85.77	15.00
100	PRO	CG	-14.82	-20.73	85.09	15.00
100	PRO	C	-18.40	-20.36	85.82	15.00
100	PRO	O	-19.33	-21.16	85.93	15.00
101	THR	N	-18.37	-19.19	86.44	15.00
101	THR	CA	-19.44	-18.75	87.32	15.00
101	THR	CB	-19.06	-17.44	88.03	15.00
101	THR	OG1	-17.64	-17.23	87.93	15.00
101	THR	CG2	-19.46	-17.51	89.50	15.00
101	THR	C	-20.74	-18.53	86.56	15.00
101	THR	O	-21.82	-18.83	87.07	15.00
102	GLY	N	-20.64	-18.01	85.35	15.00
102	GLY	CA	-21.85	-17.75	84.58	15.00
102	GLY	C	-22.38	-18.91	83.77	15.00
102	GLY	O	-23.27	-18.70	82.94	15.00
103	LYS	N	-21.85	-20.12	83.98	15.00
103	LYS	CA	-22.32	-21.28	83.21	15.00
103	LYS	CB	-21.62	-22.56	83.63	15.00
103	LYS	CG	-22.20	-23.22	84.86	15.00
103	LYS	CD	-21.67	-24.63	85.01	15.00
103	LYS	CE	-22.02	-25.45	83.79	15.00
103	LYS	NZ	-23.49	-25.45	83.60	15.00
103	LYS	C	-23.83	-21.40	83.35	15.00
103	LYS	O	-24.37	-21.25	84.45	15.00
104	ALA	N	-24.51	-21.65	82.24	15.00
104	ALA	CA	-25.96	-21.74	82.28	15.00
104	ALA	CB	-26.57	-20.48	81.67	15.00
104	ALA	C	-26.55	-22.97	81.62	15.00
104	ALA	O	-27.76	-23.22	81.72	15.00
105	ALA	N	-25.70	-23.76	80.97	15.00
105	ALA	CA	-26.17	-24.96	80.31	15.00
105	ALA	CB	-26.66	-24.65	78.91	15.00
105	ALA	C	-25.10	-26.02	80.24	15.00
105	ALA	O	-23.91	-25.72	80.09	15.00
106	LYS	N	-25.53	-27.26	80.40	15.00
106	LYS	CA	-24.65	-28.41	80.36	15.00
106	LYS	CB	-24.77	-29.23	81.64	15.00
106	LYS	CG	-24.05	-28.65	82.83	15.00
106	LYS	CD	-22.56	-28.96	82.80	15.00
106	LYS	CE	-22.28	-30.46	82.89	15.00
106	LYS	NZ	-22.56	-31.21	81.62	15.00

106 LYS C	-25.08	-29.23	79.17	15.00
106 LYS O	-26.18	-29.04	78.65	15.00
107 CYS N	-24.23	-30.15	78.76	15.00
107 CYS CA	-24.52	-31.01	77.62	15.00
107 CYS CB	-24.00	-30.36	76.33	15.00
107 CYS SG	-24.10	-31.36	74.81	15.00
107 CYS C	-23.81	-32.31	77.94	15.00
107 CYS O	-22.94	-32.34	78.81	15.00
108 ARG N	-24.23	-33.40	77.30	15.00
108 ARG CA	-23.60	-34.70	77.51	15.00
108 ARG CB	-24.27	-35.46	78.66	15.00
108 ARG CG	-25.67	-35.93	78.35	15.00
108 ARG CD	-26.16	-36.95	79.38	15.00
108 ARG NE	-27.36	-37.64	78.90	15.00
108 ARG CZ	-27.34	-38.78	78.20	15.00
108 ARG NH1	-26.18	-39.37	77.92	15.00
108 ARG NH2	-28.48	-39.29	77.75	15.00
108 ARG C	-23.57	-35.53	76.23	15.00
108 ARG O	-23.71	-36.76	76.27	15.00
109 GLY N	-23.37	-34.87	75.10	15.00
109 GLY CA	-23.30	-35.59	73.85	15.00
109 GLY C	-24.02	-34.85	72.75	15.00
109 GLY O	-24.50	-33.73	72.95	15.00
110 TYR N	-24.10	-35.48	71.59	15.00
110 TYR CA	-24.77	-34.92	70.44	15.00
110 TYR CB	-23.91	-33.89	69.74	15.00
110 TYR CG	-22.68	-34.45	69.05	15.00
110 TYR CD1	-21.45	-34.47	69.70	15.00
110 TYR CE1	-20.31	-34.89	69.04	15.00
110 TYR CD2	-22.74	-34.88	67.73	15.00
110 TYR CE2	-21.61	-35.30	67.07	15.00
110 TYR CZ	-20.39	-35.30	67.72	15.00
110 TYR OH	-19.24	-35.68	67.05	15.00
110 TYR C	-25.16	-36.02	69.48	15.00
110 TYR O	-24.41	-36.99	69.31	15.00
111 ARG N	-26.32	-35.87	68.86	15.00
111 ARG CA	-26.83	-36.84	67.91	15.00
111 ARG CB	-28.14	-37.43	68.41	15.00
111 ARG CG	-28.01	-38.15	69.74	15.00
111 ARG CD	-28.52	-39.57	69.65	15.00
111 ARG NE	-27.97	-40.28	68.49	15.00
111 ARG CZ	-28.38	-41.48	68.10	15.00

111 ARG NH1	-27.83	-42.06	67.03	15.00
111 ARG NH2	-29.32	-42.12	68.78	15.00
111 ARG C	-27.01	-36.25	66.52	15.00
111 ARG O	-27.32	-35.07	66.39	15.00
112 GLU N	-26.81	-37.06	65.50	15.00
112 GLU CA	-26.94	-36.62	64.12	15.00
112 GLU CB	-25.68	-36.90	63.30	15.00
112 GLU CG	-24.42	-36.10	63.68	15.00
112 GLU CD	-23.23	-36.42	62.77	15.00
112 GLU OE1	-22.07	-36.07	63.13	15.00
112 GLU OE2	-23.44	-37.01	61.69	15.00
112 GLU C	-28.14	-37.26	63.44	15.00
112 GLU O	-28.60	-38.33	63.84	15.00
113 ILE N	-28.61	-36.60	62.39	15.00
113 ILE CA	-29.74	-37.06	61.60	15.00
113 ILE CB	-30.51	-35.84	61.05	15.00
113 ILE CG2	-31.61	-36.25	60.09	15.00
113 ILE CG1	-31.10	-35.06	62.22	15.00
113 ILE CD1	-32.01	-35.89	63.07	15.00
113 ILE C	-29.15	-37.84	60.43	15.00
113 ILE O	-28.13	-37.44	59.88	15.00
114 PRO N	-29.74	-38.99	60.08	15.00
114 PRO CD	-30.93	-39.67	60.65	15.00
114 PRO CA	-29.19	-39.76	58.95	15.00
114 PRO CB	-30.23	-40.86	58.75	15.00
114 PRO CG	-30.78	-41.07	60.12	15.00
114 PRO C	-29.18	-38.82	57.75	15.00
114 PRO O	-30.23	-38.35	57.30	15.00
115 GLU N	-27.98	-38.53	57.25	15.00
115 GLU CA	-27.81	-37.64	56.11	15.00
115 GLU CB	-26.36	-37.71	55.63	15.00
115 GLU CG	-26.00	-38.96	54.84	15.00
115 GLU CD	-26.11	-38.74	53.34	15.00
115 GLU OE1	-26.79	-39.55	52.65	15.00
115 GLU OE2	-25.52	-37.74	52.85	15.00
115 GLU C	-28.81	-37.80	54.96	15.00
115 GLU O	-28.93	-38.86	54.37	15.00
116 GLY N	-29.54	-36.73	54.67	15.00
116 GLY CA	-30.51	-36.71	53.59	15.00
116 GLY C	-31.88	-37.25	53.92	15.00
116 GLY O	-32.76	-37.31	53.05	15.00
117 ASN N	-32.09	-37.61	55.18	15.00

117 ASN CA	-33.37	-38.18	55.61	15.00
117 ASN CB	-33.13	-39.38	56.52	15.00
117 ASN CG	-34.42	-40.02	57.01	15.00
117 ASN OD1	-35.53	-39.60	56.65	15.00
117 ASN ND2	-34.28	-41.06	57.83	15.00
117 ASN C	-34.32	-37.19	56.27	15.00
117 ASN O	-34.40	-37.10	57.50	15.00
118 GLU N	-35.10	-36.50	55.45	15.00
118 GLU CA	-36.05	-35.52	55.96	15.00
118 GLU CB	-36.81	-34.85	54.83	15.00
118 GLU CG	-36.06	-33.74	54.15	15.00
118 GLU CD	-36.96	-32.95	53.26	15.00
118 GLU OE1	-37.20	-33.39	52.11	15.00
118 GLU OE2	-37.46	-31.91	53.72	15.00
118 GLU C	-37.03	-36.09	56.96	15.00
118 GLU O	-37.48	-35.39	57.88	15.00
119 LYS N	-37.39	-37.36	56.79	15.00
119 LYS CA	-38.33	-37.99	57.71	15.00
119 LYS CB	-38.85	-39.30	57.15	15.00
119 LYS CG	-40.37	-39.34	57.05	15.00
119 LYS CD	-40.95	-38.10	56.34	15.00
119 LYS CE	-42.47	-38.10	56.44	15.00
119 LYS NZ	-43.07	-36.84	55.99	15.00
119 LYS C	-37.71	-38.16	59.09	15.00
119 LYS O	-38.36	-37.86	60.09	15.00
120 ALA N	-36.45	-38.57	59.15	15.00
120 ALA CA	-35.77	-38.75	60.44	15.00
120 ALA CB	-34.45	-39.45	60.27	15.00
120 ALA C	-35.56	-37.40	61.08	15.00
120 ALA O	-35.41	-37.31	62.30	15.00
121 LEU N	-35.52	-36.34	60.26	15.00
121 LEU CA	-35.37	-34.98	60.78	15.00
121 LEU CB	-34.93	-33.98	59.69	15.00
121 LEU CG	-34.71	-32.55	60.19	15.00
121 LEU CD1	-33.44	-32.47	61.03	15.00
121 LEU CD2	-34.62	-31.58	59.02	15.00
121 LEU C	-36.70	-34.57	61.37	15.00
121 LEU O	-36.77	-34.00	62.45	15.00
122 LYS N	-37.77	-34.88	60.65	15.00
122 LYS CA	-39.12	-34.58	61.09	15.00
122 LYS CB	-40.14	-35.16	60.12	15.00
122 LYS CG	-41.58	-34.91	60.49	15.00

122	LYS	CD	-42.51	-35.55	59.48	15.00
122	LYS	CE	-43.96	-35.15	59.73	15.00
122	LYS	NZ	-44.83	-35.53	58.58	15.00
122	LYS	C	-39.29	-35.19	62.48	15.00
122	LYS	O	-39.68	-34.50	63.42	15.00
123	ARG	N	-38.95	-36.47	62.59	15.00
123	ARG	CA	-39.04	-37.19	63.86	15.00
123	ARG	CB	-38.64	-38.65	63.70	15.00
123	ARG	CG	-39.66	-39.49	62.94	15.00
123	ARG	CD	-39.69	-40.93	63.45	15.00
123	ARG	NE	-38.49	-41.71	63.12	15.00
123	ARG	CZ	-38.54	-42.87	62.47	15.00
123	ARG	NH1	-39.71	-43.37	62.09	15.00
123	ARG	NH2	-37.42	-43.54	62.20	15.00
123	ARG	C	-38.19	-36.51	64.93	15.00
123	ARG	O	-38.63	-36.34	66.05	15.00
124	ALA	N	-36.98	-36.12	64.57	15.00
124	ALA	CA	-36.09	-35.45	65.50	15.00
124	ALA	CB	-34.77	-35.16	64.86	15.00
124	ALA	C	-36.70	-34.15	66.00	15.00
124	ALA	O	-36.77	-33.93	67.21	15.00
125	VAL	N	-37.14	-33.31	65.08	15.00
125	VAL	CA	-37.72	-32.03	65.45	15.00
125	VAL	CB	-38.13	-31.20	64.21	15.00
125	VAL	CG1	-38.87	-29.94	64.63	15.00
125	VAL	CG2	-36.90	-30.81	63.41	15.00
125	VAL	C	-38.90	-32.21	66.39	15.00
125	VAL	O	-39.02	-31.48	67.36	15.00
126	ALA	N	-39.75	-33.20	66.13	15.00
126	ALA	CA	-40.92	-33.43	66.99	15.00
126	ALA	CB	-41.96	-34.25	66.25	15.00
126	ALA	C	-40.58	-34.09	68.33	15.00
126	ALA	O	-41.09	-33.68	69.38	15.00
127	ARG	N	-39.75	-35.12	68.30	15.00
127	ARG	CA	-39.38	-35.83	69.52	15.00
127	ARG	CB	-38.82	-37.21	69.20	15.00
127	ARG	CG	-39.74	-38.08	68.36	15.00
127	ARG	CD	-39.22	-39.50	68.39	15.00
127	ARG	NE	-39.68	-40.36	67.30	15.00
127	ARG	CZ	-40.95	-40.55	66.96	15.00
127	ARG	NH1	-41.25	-41.36	65.96	15.00
127	ARG	NH2	-41.92	-39.90	67.59	15.00

127 ARG C	-38.41	-35.07	70.40	15.00
127 ARG O	-38.63	-34.94	71.60	15.00
128 VAL N	-37.33	-34.58	69.81	15.00
128 VAL CA	-36.30	-33.85	70.54	15.00
128 VAL CB	-34.95	-33.96	69.83	15.00
128 VAL CG1	-33.89	-33.20	70.59	15.00
128 VAL CG2	-34.56	-35.42	69.68	15.00
128 VAL C	-36.62	-32.39	70.77	15.00
128 VAL O	-36.73	-31.94	71.90	15.00
129 GLY N	-36.70	-31.64	69.68	15.00
129 GLY CA	-36.98	-30.21	69.76	15.00
129 GLY C	-36.20	-29.51	68.66	15.00
129 GLY O	-35.93	-30.12	67.63	15.00
130 PRO N	-35.81	-28.24	68.86	15.00
130 PRO CD	-36.15	-27.39	70.00	15.00
130 PRO CA	-35.06	-27.48	67.86	15.00
130 PRO CB	-34.77	-26.18	68.58	15.00
130 PRO CG	-36.00	-26.00	69.41	15.00
130 PRO C	-33.78	-28.20	67.49	15.00
130 PRO O	-32.98	-28.51	68.37	15.00
131 VAL N	-33.60	-28.46	66.19	15.00
131 VAL CA	-32.42	-29.16	65.69	15.00
131 VAL CB	-32.80	-30.40	64.82	15.00
131 VAL CG1	-31.55	-31.10	64.33	15.00
131 VAL CG2	-33.66	-31.37	65.60	15.00
131 VAL C	-31.54	-28.26	64.83	15.00
131 VAL O	-32.02	-27.54	63.96	15.00
132 SER N	-30.24	-28.35	65.05	15.00
132 SER CA	-29.27	-27.55	64.31	15.00
132 SER CB	-27.93	-27.54	65.04	15.00
132 SER OG	-28.09	-27.80	66.43	15.00
132 SER C	-29.11	-28.11	62.90	15.00
132 SER O	-28.80	-29.29	62.74	15.00
133 VAL N	-29.34	-27.29	61.88	15.00
133 VAL CA	-29.20	-27.74	60.49	15.00
133 VAL CB	-30.57	-27.83	59.76	15.00
133 VAL CG1	-31.29	-29.10	60.15	15.00
133 VAL CG2	-31.42	-26.63	60.06	15.00
133 VAL C	-28.26	-26.86	59.67	15.00
133 VAL O	-27.82	-25.81	60.14	15.00
134 ALA N	-27.93	-27.29	58.46	15.00
134 ALA CA	-27.05	-26.53	57.59	15.00

134 ALA CB	-25.65	-27.10	57.62	15.00
134 ALA C	-27.62	-26.60	56.18	15.00
134 ALA O	-27.92	-27.68	55.69	15.00
135 ILE N	-27.80	-25.44	55.56	15.00
135 ILE CA	-28.36	-25.36	54.21	15.00
135 ILE CB	-29.74	-24.70	54.21	15.00
135 ILE CG2	-30.76	-25.58	54.87	15.00
135 ILE CG1	-29.64	-23.31	54.87	15.00
135 ILE CD1	-30.91	-22.52	54.84	15.00
135 ILE C	-27.51	-24.50	53.29	15.00
135 ILE O	-26.46	-23.99	53.67	15.00
136 ASP N	-28.04	-24.32	52.09	15.00
136 ASP CA	-27.44	-23.50	51.05	15.00
136 ASP CB	-27.56	-24.20	49.70	15.00
136 ASP CG	-27.01	-23.38	48.56	15.00
136 ASP OD1	-27.62	-23.39	47.48	15.00
136 ASP OD2	-25.96	-22.75	48.73	15.00
136 ASP C	-28.17	-22.15	51.05	15.00
136 ASP O	-29.30	-22.07	50.57	15.00
137 ALA N	-27.56	-21.12	51.62	15.00
137 ALA CA	-28.19	-19.81	51.68	15.00
137 ALA CB	-28.23	-19.33	53.12	15.00
137 ALA C	-27.52	-18.76	50.80	15.00
137 ALA O	-27.74	-17.56	50.97	15.00
138 SER N	-26.72	-19.22	49.84	15.00
138 SER CA	-26.00	-18.34	48.92	15.00
138 SER CB	-24.80	-19.07	48.33	15.00
138 SER OG	-25.20	-20.25	47.66	15.00
138 SER C	-26.85	-17.71	47.82	15.00
138 SER O	-26.50	-16.66	47.27	15.00
139 LEU N	-27.96	-18.36	47.45	15.00
139 LEU CA	-28.85	-17.84	46.42	15.00
139 LEU CB	-29.97	-18.82	46.10	15.00
139 LEU CG	-29.63	-20.08	45.32	15.00
139 LEU CD1	-30.91	-20.89	45.13	15.00
139 LEU CD2	-29.04	-19.71	43.97	15.00
139 LEU C	-29.45	-16.51	46.85	15.00
139 LEU O	-29.82	-16.33	48.00	15.00
140 THR N	-29.61	-15.59	45.90	15.00
140 THR CA	-30.17	-14.28	46.20	15.00
140 THR CB	-29.95	-13.25	45.03	15.00
140 THR OG1	-29.88	-13.93	43.77	15.00

140	THR	CG2	-28.67	-12.47	45.23	15.00
140	THR	C	-31.65	-14.34	46.59	15.00
140	THR	O	-32.12	-13.52	47.37	15.00
141	SER	N	-32.37	-15.35	46.10	15.00
141	SER	CA	-33.79	-15.49	46.43	15.00
141	SER	CB	-34.47	-16.53	45.55	15.00
141	SER	OG	-33.70	-17.71	45.45	15.00
141	SER	C	-34.00	-15.80	47.91	15.00
141	SER	O	-34.99	-15.38	48.50	15.00
142	PHE	N	-33.07	-16.54	48.49	15.00
142	PHE	CA	-33.13	-16.89	49.91	15.00
142	PHE	CB	-32.01	-17.88	50.28	15.00
142	PHE	CG	-31.93	-18.18	51.75	15.00
142	PHE	CD1	-32.67	-19.22	52.31	15.00
142	PHE	CD2	-31.12	-17.42	52.59	15.00
142	PHE	CE1	-32.62	-19.48	53.68	15.00
142	PHE	CE2	-31.06	-17.68	53.95	15.00
142	PHE	CZ	-31.81	-18.71	54.51	15.00
142	PHE	C	-33.00	-15.60	50.70	15.00
142	PHE	O	-33.80	-15.30	51.59	15.00
143	GLN	N	-32.00	-14.81	50.30	15.00
143	GLN	CA	-31.67	-13.54	50.93	15.00
143	GLN	CB	-30.35	-13.03	50.36	15.00
143	GLN	CG	-29.20	-13.96	50.70	15.00
143	GLN	CD	-27.93	-13.71	49.91	15.00
143	GLN	OE1	-27.22	-12.73	50.12	15.00
143	GLN	NE2	-27.63	-14.63	49.01	15.00
143	GLN	C	-32.77	-12.47	50.94	15.00
143	GLN	O	-32.99	-11.82	51.97	15.00
144	PHE	N	-33.47	-12.27	49.82	15.00
144	PHE	CA	-34.54	-11.27	49.79	15.00
144	PHE	CB	-34.55	-10.47	48.49	15.00
144	PHE	CG	-34.68	-11.30	47.25	15.00
144	PHE	CD1	-33.69	-11.28	46.28	15.00
144	PHE	CD2	-35.81	-12.07	47.03	15.00
144	PHE	CE1	-33.82	-12.00	45.10	15.00
144	PHE	CE2	-35.95	-12.79	45.85	15.00
144	PHE	CZ	-34.95	-12.76	44.89	15.00
144	PHE	C	-35.92	-11.84	50.10	15.00
144	PHE	O	-36.95	-11.28	49.70	15.00
145	TYR	N	-35.94	-12.99	50.77	15.00
145	TYR	CA	-37.17	-13.65	51.15	15.00

145	TYR	CB	-36.88	-15.04	51.74	15.00
145	TYR	CG	-38.04	-15.65	52.51	15.00
145	TYR	CD1	-38.88	-16.58	51.91	15.00
145	TYR	CE1	-39.95	-17.13	52.62	15.00
145	TYR	CD2	-38.29	-15.28	53.83	15.00
145	TYR	CE2	-39.35	-15.82	54.53	15.00
145	TYR	CZ	-40.17	-16.74	53.93	15.00
145	TYR	OH	-41.23	-17.25	54.64	15.00
145	TYR	C	-37.88	-12.76	52.15	15.00
145	TYR	O	-37.25	-12.09	52.96	15.00
146	SER	N	-39.21	-12.78	52.12	15.00
146	SER	CA	-40.01	-12.00	53.04	15.00
146	SER	CB	-40.30	-10.61	52.47	15.00
146	SER	OG	-40.96	-10.71	51.22	15.00
146	SER	C	-41.29	-12.72	53.43	15.00
146	SER	O	-41.83	-12.48	54.51	15.00
147	LYS	N	-41.76	-13.63	52.58	15.00
147	LYS	CA	-42.98	-14.39	52.86	15.00
147	LYS	CB	-44.22	-13.50	52.79	15.00
147	LYS	CG	-44.61	-13.04	51.39	15.00
147	LYS	CD	-45.75	-12.03	51.44	15.00
147	LYS	CE	-45.98	-11.35	50.09	15.00
147	LYS	NZ	-47.01	-10.28	50.19	15.00
147	LYS	C	-43.16	-15.60	51.95	15.00
147	LYS	O	-42.49	-15.70	50.92	15.00
148	GLY	N	-44.05	-16.50	52.36	15.00
148	GLY	CA	-44.34	-17.71	51.60	15.00
148	GLY	C	-43.51	-18.90	52.07	15.00
148	GLY	O	-42.99	-18.90	53.18	15.00
149	VAL	N	-43.43	-19.92	51.22	15.00
149	VAL	CA	-42.66	-21.12	51.51	15.00
149	VAL	CB	-43.53	-22.39	51.40	15.00
149	VAL	CG1	-42.69	-23.64	51.56	15.00
149	VAL	CG2	-44.62	-22.35	52.45	15.00
149	VAL	C	-41.53	-21.16	50.47	15.00
149	VAL	O	-41.75	-21.48	49.30	15.00
150	TYR	N	-40.33	-20.80	50.90	15.00
150	TYR	CA	-39.19	-20.78	50.01	15.00
150	TYR	CB	-37.96	-20.25	50.75	15.00
150	TYR	CG	-36.72	-20.12	49.90	15.00
150	TYR	CD1	-36.64	-19.13	48.91	15.00
150	TYR	CE1	-35.51	-19.02	48.09	15.00

150 TYR CD2	-35.64	-20.99	50.05	15.00
150 TYR CE2	-34.51	-20.89	49.24	15.00
150 TYR CZ	-34.45	-19.91	48.26	15.00
150 TYR OH	-33.36	-19.82	47.42	15.00
150 TYR C	-38.89	-22.11	49.33	15.00
150 TYR O	-38.81	-23.15	49.98	15.00
151 TYR N	-38.77	-22.06	48.01	15.00
151 TYR CA	-38.39	-23.22	47.21	15.00
151 TYR CB	-39.55	-24.11	46.79	15.00
151 TYR CG	-39.06	-25.31	45.98	15.00
151 TYR CD1	-37.99	-26.08	46.43	15.00
151 TYR CE1	-37.47	-27.12	45.66	15.00
151 TYR CD2	-39.60	-25.61	44.73	15.00
151 TYR CE2	-39.09	-26.64	43.95	15.00
151 TYR CZ	-38.02	-27.39	44.43	15.00
151 TYR OH	-37.46	-28.37	43.65	15.00
151 TYR C	-37.65	-22.71	45.98	15.00
151 TYR O	-38.13	-21.81	45.29	15.00
152 ASP N	-36.50	-23.30	45.71	15.00
152 ASP CA	-35.69	-22.88	44.58	15.00
152 ASP CB	-34.92	-21.62	44.94	15.00
152 ASP CG	-34.31	-20.95	43.75	15.00
152 ASP OD1	-33.30	-21.46	43.24	15.00
152 ASP OD2	-34.83	-19.90	43.34	15.00
152 ASP C	-34.74	-24.00	44.16	15.00
152 ASP O	-33.67	-24.16	44.74	15.00
153 GLU N	-35.12	-24.77	43.14	15.00
153 GLU CA	-34.30	-25.88	42.66	15.00
153 GLU CB	-34.99	-26.68	41.55	15.00
153 GLU CG	-35.86	-25.85	40.61	15.00
153 GLU CD	-35.20	-24.55	40.21	15.00
153 GLU OE1	-35.85	-23.49	40.40	15.00
153 GLU OE2	-34.05	-24.58	39.73	15.00
153 GLU C	-32.88	-25.53	42.24	15.00
153 GLU O	-32.12	-26.41	41.84	15.00
154 SER N	-32.56	-24.24	42.24	15.00
154 SER CA	-31.21	-23.81	41.87	15.00
154 SER CB	-31.23	-22.38	41.29	15.00
154 SER OG	-29.99	-22.04	40.68	15.00
154 SER C	-30.32	-23.92	43.11	15.00
154 SER O	-29.08	-23.86	43.03	15.00
155 CYS N	-30.95	-24.11	44.26	15.00

155 CYS CA	-30.25	-24.27	45.52	15.00
155 CYS C	-29.46	-25.57	45.44	15.00
155 CYS O	-30.01	-26.60	45.04	15.00
155 CYS CB	-31.24	-24.29	46.67	15.00
155 CYS SG	-30.52	-24.05	48.32	15.00
156 ASN N	-28.18	-25.54	45.80	15.00
156 ASN CA	-27.32	-26.73	45.73	15.00
156 ASN CB	-25.94	-26.34	45.18	15.00
156 ASN CG	-25.00	-27.52	45.10	15.00
156 ASN OD1	-25.41	-28.68	45.25	15.00
156 ASN ND2	-23.72	-27.24	44.86	15.00
156 ASN C	-27.17	-27.54	47.03	15.00
156 ASN O	-26.43	-27.15	47.94	15.00
157 SER N	-27.79	-28.71	47.05	15.00
157 SER CA	-27.75	-29.59	48.22	15.00
157 SER CB	-28.54	-30.87	47.97	15.00
157 SER OG	-29.86	-30.55	47.53	15.00
157 SER C	-26.34	-29.93	48.65	15.00
157 SER O	-26.09	-30.17	49.82	15.00
158 ASP N	-25.42	-29.97	47.69	15.00
158 ASP CA	-24.04	-30.32	47.98	15.00
158 ASP CB	-23.39	-30.98	46.77	15.00
158 ASP CG	-24.30	-32.01	46.10	15.00
158 ASP OD1	-25.16	-31.59	45.30	15.00
158 ASP OD2	-24.16	-33.22	46.38	15.00
158 ASP C	-23.23	-29.12	48.47	15.00
158 ASP O	-22.07	-29.26	48.88	15.00
159 ASN N	-23.84	-27.94	48.44	15.00
159 ASN CA	-23.16	-26.74	48.87	15.00
159 ASN CB	-23.23	-25.65	47.79	15.00
159 ASN CG	-22.43	-24.40	48.16	15.00
159 ASN OD1	-21.20	-24.43	48.25	15.00
159 ASN ND2	-23.13	-23.30	48.37	15.00
159 ASN C	-23.72	-26.25	50.20	15.00
159 ASN O	-24.52	-25.31	50.24	15.00
160 LEU N	-23.32	-26.89	51.29	15.00
160 LEU CA	-23.78	-26.48	52.62	15.00
160 LEU CB	-23.80	-27.66	53.59	15.00
160 LEU CG	-24.71	-28.86	53.26	15.00
160 LEU CD1	-24.59	-29.92	54.34	15.00
160 LEU CD2	-26.15	-28.43	53.10	15.00
160 LEU C	-22.89	-25.34	53.12	15.00

160 LEU O	-21.71	-25.55	53.43	15.00
161 ASN N	-23.46	-24.15	53.23	15.00
161 ASN CA	-22.70	-22.98	53.65	15.00
161 ASN CB	-22.49	-22.04	52.46	15.00
161 ASN CG	-23.80	-21.60	51.80	15.00
161 ASN OD1	-24.62	-20.89	52.40	15.00
161 ASN ND2	-24.02	-22.04	50.57	15.00
161 ASN C	-23.24	-22.19	54.82	15.00
161 ASN O	-22.50	-21.41	55.44	15.00
162 HIS N	-24.50	-22.38	55.16	15.00
162 HIS CA	-25.09	-21.63	56.25	15.00
162 HIS CB	-26.09	-20.60	55.70	15.00
162 HIS CG	-26.36	-19.45	56.63	15.00
162 HIS CD2	-27.52	-18.88	57.02	15.00
162 HIS ND1	-25.35	-18.74	57.27	15.00
162 HIS CE1	-25.89	-17.79	58.01	15.00
162 HIS NE2	-27.20	-17.85	57.88	15.00
162 HIS C	-25.73	-22.52	57.32	15.00
162 HIS O	-26.57	-23.36	57.03	15.00
163 ALA N	-25.29	-22.33	58.56	15.00
163 ALA CA	-25.82	-23.08	59.68	15.00
163 ALA CB	-24.83	-23.11	60.82	15.00
163 ALA C	-27.09	-22.35	60.10	15.00
163 ALA O	-27.17	-21.12	60.04	15.00
164 VAL N	-28.07	-23.10	60.57	15.00
164 VAL CA	-29.33	-22.51	60.95	15.00
164 VAL CB	-30.15	-22.28	59.67	15.00
164 VAL CG1	-30.99	-23.50	59.31	15.00
164 VAL CG2	-30.94	-21.02	59.76	15.00
164 VAL C	-30.02	-23.41	62.00	15.00
164 VAL O	-29.40	-24.32	62.53	15.00
165 LEU N	-31.28	-23.14	62.31	15.00
165 LEU CA	-31.97	-23.95	63.31	15.00
165 LEU CB	-31.89	-23.27	64.69	15.00
165 LEU CG	-32.54	-23.86	65.94	15.00
165 LEU CD1	-31.64	-24.89	66.56	15.00
165 LEU CD2	-32.80	-22.75	66.92	15.00
165 LEU C	-33.42	-24.23	62.94	15.00
165 LEU O	-34.17	-23.31	62.68	15.00
166 ALA N	-33.78	-25.51	62.87	15.00
166 ALA CA	-35.16	-25.91	62.55	15.00
166 ALA CB	-35.20	-27.32	62.01	15.00

166 ALA C	-35.95	-25.80	63.83	15.00
166 ALA O	-35.67	-26.47	64.81	15.00
167 VAL N	-36.93	-24.91	63.82	15.00
167 VAL CA	-37.77	-24.62	64.97	15.00
167 VAL CB	-37.87	-23.05	65.10	15.00
167 VAL CG1	-39.11	-22.60	65.81	15.00
167 VAL CG2	-36.64	-22.53	65.82	15.00
167 VAL C	-39.14	-25.30	64.88	15.00
167 VAL O	-39.98	-25.17	65.77	15.00
168 GLY N	-39.36	-26.05	63.81	15.00
168 GLY CA	-40.63	-26.73	63.66	15.00
168 GLY C	-40.88	-27.11	62.23	15.00
168 GLY O	-39.96	-27.09	61.41	15.00
169 TYR N	-42.12	-27.45	61.92	15.00
169 TYR CA	-42.52	-27.84	60.57	15.00
169 TYR CB	-41.99	-29.24	60.21	15.00
169 TYR CG	-42.49	-30.37	61.09	15.00
169 TYR CD1	-43.82	-30.80	61.01	15.00
169 TYR CE1	-44.30	-31.81	61.82	15.00
169 TYR CD2	-41.66	-30.99	62.01	15.00
169 TYR CE2	-42.13	-32.01	62.83	15.00
169 TYR CZ	-43.46	-32.41	62.73	15.00
169 TYR OH	-43.96	-33.41	63.53	15.00
169 TYR C	-44.03	-27.76	60.48	15.00
169 TYR O	-44.71	-27.65	61.49	15.00
170 GLY N	-44.57	-27.80	59.26	15.00
170 GLY CA	-46.01	-27.72	59.11	15.00
170 GLY C	-46.48	-27.54	57.68	15.00
170 GLY O	-45.85	-28.04	56.75	15.00
171 ILE N	-47.55	-26.79	57.50	15.00
171 ILE CA	-48.11	-26.53	56.18	15.00
171 ILE CB	-49.30	-27.48	55.85	15.00
171 ILE CG2	-48.79	-28.88	55.55	15.00
171 ILE CG1	-50.29	-27.53	57.02	15.00
171 ILE CD1	-51.40	-26.48	56.97	15.00
171 ILE C	-48.63	-25.10	56.07	15.00
171 ILE O	-48.87	-24.44	57.08	15.00
172 GLN N	-48.75	-24.62	54.84	15.00
172 GLN CA	-49.27	-23.28	54.60	15.00
172 GLN CB	-48.22	-22.34	54.00	15.00
172 GLN CG	-48.63	-20.86	53.96	15.00
172 GLN CD	-47.49	-19.92	54.36	15.00

172 GLN OE1	-47.54	-19.28	55.40	15.00
172 GLN NE2	-46.46	-19.83	53.52	15.00
172 GLN C	-50.46	-23.45	53.67	15.00
172 GLN O	-51.49	-24.00	54.07	15.00
173 LYS N	-50.30	-23.07	52.41	15.00
173 LYS CA	-51.38	-23.21	51.46	15.00
173 LYS CB	-51.36	-22.10	50.42	15.00
173 LYS CG	-51.38	-20.70	51.04	15.00
173 LYS CD	-52.68	-20.45	51.78	15.00
173 LYS CE	-53.81	-20.28	50.78	15.00
173 LYS NZ	-53.58	-19.10	49.88	15.00
173 LYS C	-51.15	-24.57	50.86	15.00
173 LYS O	-50.84	-24.70	49.68	15.00
174 GLY N	-51.19	-25.57	51.73	15.00
174 GLY CA	-50.98	-26.94	51.31	15.00
174 GLY C	-49.52	-27.32	51.13	15.00
174 GLY O	-49.20	-28.49	50.87	15.00
175 ASN N	-48.63	-26.35	51.27	15.00
175 ASN CA	-47.21	-26.62	51.11	15.00
175 ASN CB	-46.45	-25.42	50.56	15.00
175 ASN CG	-47.23	-24.69	49.49	15.00
175 ASN OD1	-48.07	-23.83	49.80	15.00
175 ASN ND2	-46.97	-25.03	48.24	15.00
175 ASN C	-46.60	-27.05	52.42	15.00
175 ASN O	-46.82	-26.41	53.46	15.00
176 LYS N	-45.87	-28.16	52.38	15.00
176 LYS CA	-45.20	-28.68	53.57	15.00
176 LYS CB	-44.69	-30.10	53.34	15.00
176 LYS CG	-45.74	-31.11	52.86	15.00
176 LYS CD	-46.88	-31.26	53.85	15.00
176 LYS CE	-47.97	-32.21	53.34	15.00
176 LYS NZ	-48.80	-31.66	52.19	15.00
176 LYS C	-44.05	-27.71	53.76	15.00
176 LYS O	-43.63	-27.08	52.80	15.00
177 HIS N	-43.57	-27.54	54.99	15.00
177 HIS CA	-42.45	-26.64	55.21	15.00
177 HIS CB	-42.88	-25.18	54.99	15.00
177 HIS CG	-43.82	-24.66	56.02	15.00
177 HIS CD2	-43.66	-24.45	57.35	15.00
177 HIS ND1	-45.10	-24.21	55.71	15.00
177 HIS CE1	-45.67	-23.75	56.81	15.00
177 HIS NE2	-44.82	-23.88	57.81	15.00

177 HIS C	-41.71	-26.78	56.53	15.00
177 HIS O	-42.23	-27.35	57.50	15.00
178 TRP N	-40.49	-26.24	56.54	15.00
178 TRP CA	-39.60	-26.23	57.69	15.00
178 TRP CB	-38.19	-26.64	57.31	15.00
178 TRP CG	-37.99	-28.06	56.96	15.00
178 TRP CD2	-38.07	-29.18	57.84	15.00
178 TRP CE2	-37.75	-30.33	57.09	15.00
178 TRP CE3	-38.38	-29.33	59.20	15.00
178 TRP CD1	-37.64	-28.56	55.74	15.00
178 TRP NE1	-37.49	-29.92	55.81	15.00
178 TRP CZ2	-37.73	-31.61	57.65	15.00
178 TRP CZ3	-38.37	-30.60	59.76	15.00
178 TRP CH2	-38.05	-31.72	58.98	15.00
178 TRP C	-39.54	-24.81	58.28	15.00
178 TRP O	-39.17	-23.88	57.58	15.00
179 ILE N	-39.90	-24.63	59.55	15.00
179 ILE CA	-39.78	-23.31	60.15	15.00
179 ILE CB	-40.56	-23.19	61.47	15.00
179 ILE CG2	-40.42	-21.80	62.04	15.00
179 ILE CG1	-42.03	-23.55	61.26	15.00
179 ILE CD1	-42.83	-23.54	62.53	15.00
179 ILE C	-38.30	-23.20	60.48	15.00
179 ILE O	-37.76	-24.02	61.22	15.00
180 ILE N	-37.61	-22.23	59.88	15.00
180 ILE CA	-36.18	-22.05	60.12	15.00
180 ILE CB	-35.39	-22.09	58.78	15.00
180 ILE CG2	-33.93	-21.75	58.98	15.00
180 ILE CG1	-35.49	-23.48	58.17	15.00
180 ILE CD1	-35.01	-24.57	59.10	15.00
180 ILE C	-35.91	-20.73	60.84	15.00
180 ILE O	-36.58	-19.74	60.60	15.00
181 LYS N	-34.98	-20.76	61.79	15.00
181 LYS CA	-34.59	-19.57	62.52	15.00
181 LYS CB	-34.57	-19.82	64.03	15.00
181 LYS CG	-34.13	-18.62	64.86	15.00
181 LYS CD	-33.87	-19.01	66.30	15.00
181 LYS CE	-33.59	-17.80	67.13	15.00
181 LYS NZ	-33.32	-18.14	68.55	15.00
181 LYS C	-33.19	-19.24	62.02	15.00
181 LYS O	-32.27	-20.05	62.15	15.00
182 ASN N	-33.04	-18.08	61.38	15.00

182 ASN CA	-31.75	-17.66	60.85	15.00
182 ASN CB	-31.93	-16.90	59.53	15.00
182 ASN CG	-30.71	-16.97	58.64	15.00
182 ASN OD1	-29.58	-17.07	59.11	15.00
182 ASN ND2	-30.94	-16.92	57.33	15.00
182 ASN C	-31.07	-16.80	61.91	15.00
182 ASN O	-31.52	-16.75	63.05	15.00
183 SER N	-29.98	-16.13	61.55	15.00
183 SER CA	-29.28	-15.27	62.49	15.00
183 SER CB	-28.10	-16.00	63.13	15.00
183 SER OG	-27.27	-16.59	62.15	15.00
183 SER C	-28.83	-13.99	61.81	15.00
183 SER O	-27.65	-13.66	61.82	15.00
184 TRP N	-29.77	-13.30	61.17	15.00
184 TRP CA	-29.49	-12.05	60.48	15.00
184 TRP CB	-29.61	-12.22	58.96	15.00
184 TRP CG	-28.60	-13.15	58.37	15.00
184 TRP CD2	-28.66	-13.78	57.08	15.00
184 TRP CE2	-27.49	-14.55	56.94	15.00
184 TRP CE3	-29.60	-13.77	56.03	15.00
184 TRP CD1	-27.43	-13.56	58.93	15.00
184 TRP NE1	-26.76	-14.39	58.08	15.00
184 TRP CZ2	-27.22	-15.31	55.78	15.00
184 TRP CZ3	-29.33	-14.53	54.89	15.00
184 TRP CH2	-28.15	-15.29	54.78	15.00
184 TRP C	-30.42	-10.97	61.00	15.00
184 TRP O	-30.89	-10.12	60.25	15.00
185 GLY N	-30.70	-11.03	62.30	15.00
185 GLY CA	-31.58	-10.07	62.94	15.00
185 GLY C	-33.02	-10.33	62.57	15.00
185 GLY O	-33.31	-11.05	61.62	15.00
186 GLU N	-33.94	-9.76	63.35	15.00
186 GLU CA	-35.36	-9.93	63.07	15.00
186 GLU CB	-36.22	-9.59	64.28	15.00
186 GLU CG	-36.03	-8.21	64.80	15.00
186 GLU CD	-36.84	-7.96	66.04	15.00
186 GLU OE1	-37.97	-8.49	66.13	15.00
186 GLU OE2	-36.35	-7.22	66.93	15.00
186 GLU C	-35.77	-9.12	61.86	15.00
186 GLU O	-36.90	-9.24	61.38	15.00
187 ASN N	-34.84	-8.32	61.36	15.00
187 ASN CA	-35.06	-7.47	60.20	15.00

187 ASN CB	-34.05	-6.32	60.16	15.00
187 ASN CG	-34.41	-5.27	59.11	15.00
187 ASN OD1	-35.57	-5.16	58.70	15.00
187 ASN ND2	-33.41	-4.49	58.69	15.00
187 ASN C	-35.00	-8.26	58.91	15.00
187 ASN O	-35.44	-7.79	57.86	15.00
188 TRP N	-34.42	-9.46	58.97	15.00
188 TRP CA	-34.30	-10.30	57.80	15.00
188 TRP CB	-33.01	-11.12	57.86	15.00
188 TRP CG	-32.84	-11.99	56.71	15.00
188 TRP CD2	-33.26	-13.36	56.60	15.00
188 TRP CE2	-32.96	-13.77	55.29	15.00
188 TRP CE3	-33.86	-14.26	57.48	15.00
188 TRP CD1	-32.32	-11.65	55.51	15.00
188 TRP NE1	-32.39	-12.71	54.64	15.00
188 TRP CZ2	-33.24	-15.07	54.83	15.00
188 TRP CZ3	-34.15	-15.55	57.02	15.00
188 TRP CH2	-33.84	-15.94	55.72	15.00
188 TRP C	-35.50	-11.21	57.63	15.00
188 TRP O	-36.05	-11.71	58.61	15.00
189 GLY N	-35.92	-11.43	56.38	15.00
189 GLY CA	-37.05	-12.30	56.10	15.00
189 GLY C	-38.29	-11.99	56.92	15.00
189 GLY O	-38.61	-10.83	57.20	15.00
190 ASN N	-39.01	-13.04	57.31	15.00
190 ASN CA	-40.21	-12.85	58.11	15.00
190 ASN CB	-41.21	-13.98	57.90	15.00
190 ASN CG	-42.58	-13.65	58.45	15.00
190 ASN OD1	-42.74	-12.81	59.33	15.00
190 ASN ND2	-43.60	-14.32	57.92	15.00
190 ASN C	-39.77	-12.74	59.56	15.00
190 ASN O	-39.83	-13.72	60.30	15.00
191 LYS N	-39.24	-11.59	59.94	15.00
191 LYS CA	-38.80	-11.39	61.31	15.00
191 LYS CB	-40.02	-11.23	62.23	15.00
191 LYS CG	-40.86	-10.00	61.87	15.00
191 LYS CD	-42.05	-9.79	62.79	15.00
191 LYS CE	-43.16	-10.79	62.51	15.00
191 LYS NZ	-43.76	-10.63	61.14	15.00
191 LYS C	-37.83	-12.46	61.81	15.00
191 LYS O	-38.02	-13.08	62.86	15.00
192 GLY N	-36.77	-12.65	61.03	15.00

192 GLY CA	-35.73	-13.62	61.37	15.00
192 GLY C	-35.96	-15.05	60.91	15.00
192 GLY O	-35.00	-15.80	60.72	15.00
193 TYR N	-37.21	-15.43	60.71	15.00
193 TYR CA	-37.53	-16.78	60.30	15.00
193 TYR CB	-38.71	-17.32	61.10	15.00
193 TYR CG	-38.44	-17.47	62.58	15.00
193 TYR CD1	-38.48	-16.39	63.44	15.00
193 TYR CE1	-38.21	-16.54	64.79	15.00
193 TYR CD2	-38.12	-18.72	63.11	15.00
193 TYR CE2	-37.84	-18.88	64.46	15.00
193 TYR CZ	-37.89	-17.79	65.29	15.00
193 TYR OH	-37.62	-17.95	66.63	15.00
193 TYR C	-37.78	-16.91	58.82	15.00
193 TYR O	-38.05	-15.93	58.14	15.00
194 ILE N	-37.72	-18.14	58.33	15.00
194 ILE CA	-37.95	-18.43	56.92	15.00
194 ILE CB	-36.63	-18.38	56.07	15.00
194 ILE CG2	-35.63	-19.42	56.55	15.00
194 ILE CG1	-36.94	-18.61	54.60	15.00
194 ILE CD1	-35.75	-18.49	53.69	15.00
194 ILE C	-38.57	-19.82	56.79	15.00
194 ILE O	-38.12	-20.78	57.42	15.00
195 LEU N	-39.65	-19.91	56.03	15.00
195 LEU CA	-40.34	-21.17	55.80	15.00
195 LEU CB	-41.84	-20.95	55.67	15.00
195 LEU CG	-42.72	-21.15	56.90	15.00
195 LEU CD1	-42.11	-20.50	58.14	15.00
195 LEU CD2	-44.10	-20.59	56.59	15.00
195 LEU C	-39.79	-21.84	54.56	15.00
195 LEU O	-40.17	-21.50	53.45	15.00
196 MET N	-38.86	-22.76	54.75	15.00
196 MET CA	-38.25	-23.48	53.63	15.00
196 MET CB	-36.83	-23.91	53.98	15.00
196 MET CG	-35.91	-22.73	54.21	15.00
196 MET SD	-34.18	-23.17	54.37	15.00
196 MET CE	-33.94	-24.05	52.84	15.00
196 MET C	-39.13	-24.66	53.22	15.00
196 MET O	-40.03	-25.06	53.97	15.00
197 ALA N	-38.87	-25.24	52.05	15.00
197 ALA CA	-39.67	-26.35	51.54	15.00
197 ALA CB	-39.50	-26.46	50.04	15.00

197 ALA C	-39.40	-27.70	52.18	15.00
197 ALA O	-38.26	-28.15	52.25	15.00
198 ARG N	-40.47	-28.36	52.62	15.00
198 ARG CA	-40.35	-29.67	53.24	15.00
198 ARG CB	-41.11	-29.71	54.57	15.00
198 ARG CG	-41.08	-31.06	55.27	15.00
198 ARG CD	-41.32	-30.93	56.75	15.00
198 ARG NE	-42.61	-30.32	57.06	15.00
198 ARG CZ	-43.76	-30.98	57.14	15.00
198 ARG NH1	-43.79	-32.29	56.95	15.00
198 ARG NH2	-44.88	-30.33	57.45	15.00
198 ARG C	-40.82	-30.77	52.30	15.00
198 ARG O	-41.91	-30.70	51.73	15.00
199 ASN N	-39.97	-31.76	52.12	15.00
199 ASN CA	-40.27	-32.90	51.25	15.00
199 ASN CB	-41.62	-33.54	51.63	15.00
199 ASN CG	-41.53	-34.36	52.90	15.00
199 ASN OD1	-42.42	-34.31	53.75	15.00
199 ASN ND2	-40.45	-35.13	53.05	15.00
199 ASN C	-40.21	-32.59	49.76	15.00
199 ASN O	-40.78	-33.32	48.94	15.00
200 LYS N	-39.48	-31.54	49.41	15.00
200 LYS CA	-39.31	-31.17	48.01	15.00
200 LYS CB	-39.31	-29.66	47.81	15.00
200 LYS CG	-40.70	-29.02	47.77	15.00
200 LYS CD	-41.37	-29.23	46.42	15.00
200 LYS CE	-42.76	-28.59	46.37	15.00
200 LYS NZ	-42.73	-27.14	46.73	15.00
200 LYS C	-37.98	-31.78	47.60	15.00
200 LYS O	-37.11	-31.09	47.06	15.00
201 ASN N	-37.81	-33.06	47.93	15.00
201 ASN CA	-36.58	-33.78	47.62	15.00
201 ASN CB	-36.41	-33.93	46.11	15.00
201 ASN CG	-37.15	-35.13	45.56	15.00
201 ASN OD1	-36.68	-35.78	44.63	15.00
201 ASN ND2	-38.32	-35.42	46.13	15.00
201 ASN C	-35.33	-33.22	48.27	15.00
201 ASN O	-34.27	-33.16	47.66	15.00
202 ASN N	-35.46	-32.84	49.54	15.00
202 ASN CA	-34.37	-32.30	50.35	15.00
202 ASN CB	-33.25	-33.34	50.49	15.00
202 ASN CG	-32.20	-32.93	51.48	15.00

202 ASN OD1	-32.51	-32.44	52.56	15.00
202 ASN ND2	-30.94	-33.14	51.13	15.00
202 ASN C	-33.83	-30.96	49.85	15.00
202 ASN O	-32.62	-30.77	49.68	15.00
203 ALA N	-34.73	-30.00	49.69	15.00
203 ALA H	-35.60	-30.20	50.07	15.00
203 ALA CA	-34.39	-28.68	49.18	15.00
203 ALA CB	-35.57	-27.74	49.24	15.00
203 ALA C	-33.27	-28.06	50.04	15.00
203 ALA O	-33.33	-28.03	51.26	15.00
204 CYS N	-32.23	-27.56	49.35	15.00
204 CYS CA	-31.11	-26.89	50.02	15.00
204 CYS C	-30.29	-27.71	51.00	15.00
204 CYS O	-29.50	-27.14	51.76	15.00
204 CYS CB	-31.58	-25.60	50.69	15.00
204 CYS SG	-32.12	-24.29	49.55	15.00
205 GLY N	-30.43	-29.03	50.98	15.00
205 GLY CA	-29.68	-29.88	51.90	15.00
205 GLY C	-30.10	-29.71	53.35	15.00
205 GLY O	-29.31	-29.92	54.27	15.00
206 ILE N	-31.37	-29.38	53.54	15.00
206 ILE CA	-31.95	-29.16	54.85	15.00
206 ILE CB	-33.46	-28.92	54.73	15.00
206 ILE CG2	-34.13	-30.13	54.12	15.00
206 ILE CG1	-34.06	-28.55	56.10	15.00
206 ILE CD1	-33.76	-27.15	56.54	15.00
206 ILE C	-31.71	-30.29	55.85	15.00
206 ILE O	-31.47	-30.04	57.03	15.00
207 ALA N	-31.79	-31.54	55.38	15.00
207 ALA CA	-31.58	-32.69	56.25	15.00
207 ALA CB	-32.72	-33.68	56.08	15.00
207 ALA C	-30.25	-33.35	55.94	15.00
207 ALA O	-30.15	-34.57	55.95	15.00
208 ASN N	-29.24	-32.54	55.67	15.00
208 ASN CA	-27.91	-33.04	55.33	15.00
208 ASN CB	-27.41	-32.42	54.03	15.00
208 ASN CG	-27.70	-33.30	52.84	15.00
208 ASN OD1	-28.85	-33.50	52.47	15.00
208 ASN ND2	-26.65	-33.86	52.26	15.00
208 ASN C	-26.85	-32.89	56.41	15.00
208 ASN O	-25.80	-33.53	56.35	15.00
209 LEU N	-27.08	-32.00	57.36	15.00

209 LEU CA	-26.10	-31.82	58.42	15.00
209 LEU CB	-25.07	-30.77	58.03	15.00
209 LEU CG	-23.69	-31.04	58.63	15.00
209 LEU CD1	-23.08	-32.21	57.88	15.00
209 LEU CD2	-22.82	-29.81	58.52	15.00
209 LEU C	-26.77	-31.46	59.73	15.00
209 LEU O	-26.25	-30.66	60.51	15.00
210 ALA N	-27.91	-32.08	59.97	15.00
210 ALA H	-27.81	-31.90	59.38	15.00
210 ALA CA	-28.67	-31.80	61.19	15.00
210 ALA CB	-29.27	-31.17	61.33	15.00
210 ALA C	-28.06	-32.58	62.37	15.00
210 ALA O	-27.58	-33.69	62.23	15.00
211 SER N	-28.08	-31.93	63.53	15.00
211 SER CA	-27.60	-32.53	64.76	15.00
211 SER CB	-26.07	-32.52	64.86	15.00
211 SER OG	-25.53	-31.21	64.89	15.00
211 SER C	-28.25	-31.80	65.93	15.00
211 SER O	-28.68	-30.65	65.78	15.00
212 PHE N	-28.44	-32.51	67.03	15.00
212 PHE CA	-29.04	-31.94	68.23	15.00
212 PHE CB	-30.53	-32.29	68.37	15.00
212 PHE CG	-30.81	-33.77	68.41	15.00
212 PHE CD1	-31.04	-34.48	67.24	15.00
212 PHE CD2	-30.85	-34.45	69.62	15.00
212 PHE CE1	-31.30	-35.84	67.27	15.00
212 PHE CE2	-31.11	-35.82	69.67	15.00
212 PHE CZ	-31.33	-36.51	68.48	15.00
212 PHE C	-28.22	-32.41	69.43	15.00
212 PHE O	-27.54	-33.43	69.36	15.00
213 PRO N	-28.19	-31.63	70.50	15.00
213 PRO CD	-28.56	-30.21	70.63	15.00
213 PRO CA	-27.41	-32.07	71.65	15.00
213 PRO CB	-26.98	-30.75	72.28	15.00
213 PRO CG	-28.17	-29.90	72.06	15.00
213 PRO C	-28.21	-32.91	72.65	15.00
213 PRO O	-29.45	-32.81	72.72	15.00
214 LYS N	-27.50	-33.77	73.38	15.00
214 LYS CA	-28.12	-34.59	74.42	15.00
214 LYS CB	-27.50	-35.97	74.52	15.00
214 LYS CG	-28.01	-37.00	73.53	15.00
214 LYS CD	-27.20	-38.28	73.68	15.00

214 LYS CE	-27.79	-39.45	72.93	15.00
214 LYS NZ	-27.00	-40.67	73.21	15.00
214 LYS C	-27.86	-33.84	75.70	15.00
214 LYS O	-26.73	-33.45	75.98	15.00
215 MET N	-28.90	-33.63	76.49	15.00
215 MET CA	-28.73	-32.91	77.73	15.00
215 MET CB	-29.47	-31.58	77.67	15.00
215 MET CG	-28.62	-30.45	78.17	15.00
215 MET SD	-29.49	-28.92	78.17	15.00
215 MET CE	-30.02	-28.81	79.89	15.00
215 MET C	-29.15	-33.74	78.95	15.00
215 MET OT1	-30.12	-34.53	78.84	15.00
215 MET OT2	-28.49	-33.59	80.01	15.00
216 HOH OH2	-28.59	-18.05	86.43	15.00
217 HOH OH2	-24.24	-33.32	82.08	15.00
218 HOH OH2	-30.97	-16.19	65.69	15.00
219 HOH OH2	-30.10	-20.71	63.47	15.00
220 HOH OH2	-13.66	-11.12	63.10	15.00
221 HOH OH2	-9.67	-9.48	64.25	15.00
222 HOH OH2	-34.55	-23.08	70.24	15.00
223 HOH OH2	-14.15	-32.13	69.51	15.00
224 HOH OH2	-11.90	-8.52	62.51	15.00
225 HOH OH2	-24.25	-30.66	62.17	15.00
226 HOH OH2	-10.58	-2.52	79.25	15.00
227 HOH OH2	-14.05	-21.32	67.22	15.00
228 HOH OH2	-44.68	-30.63	50.04	15.00
229 HOH OH2	-45.38	-36.05	56.05	15.00
230 HOH OH2	-39.65	-13.31	65.32	15.00
231 HOH OH2	-35.12	-36.60	49.29	15.00
232 HOH OH2	-17.36	-34.13	65.07	15.00
233 HOH OH2	-30.35	-19.53	65.73	15.00
234 HOH OH2	-27.89	-19.53	62.51	15.00
235 HOH OH2	-21.85	-29.55	62.34	15.00
236 HOH OH2	-30.14	3.73	67.17	15.00
237 HOH OH2	-40.50	-29.62	80.16	15.00
238 HOH OH2	-27.85	-23.15	86.33	15.00
239 HOH OH2	-38.29	-13.95	44.87	15.00
240 HOH OH2	-36.58	-24.59	50.05	15.00
241 HOH OH2	-46.68	-34.18	57.37	15.00
242 HOH OH2	-26.77	-6.82	59.79	15.00
243 HOH OH2	-43.58	-17.40	60.45	15.00
244 HOH OH2	-23.22	-6.13	61.38	15.00

245	HOH	OH2	-33.13	-28.30	71.09	15.00
246	HOH	OH2	-46.57	-25.22	78.97	15.00
247	HOH	OH2	-14.51	-7.76	88.79	15.00
248	HOH	OH2	-3.26	-20.73	74.76	15.00
249	HOH	OH2	0.44	-15.91	75.31	15.00
250	HOH	OH2	-19.71	-34.82	58.63	15.00
251	HOH	OH2	-34.91	-11.28	53.79	15.00
252	HOH	OH2	-32.46	-28.27	46.13	15.00
253	HOH	OH2	-38.20	-15.68	37.93	15.00
254	HOH	OH2	-41.44	-34.28	56.30	15.00
255	HOH	OH2	-46.93	-13.62	73.92	15.00
256	HOH	OH2	-32.58	-13.60	60.68	15.00
257	HOH	OH2	-35.46	-6.38	55.50	15.00
258	HOH	OH2	-24.79	-7.91	66.67	15.00
259	HOH	OH2	-32.06	-6.48	63.77	15.00
260	HOH	OH2	-17.19	-5.30	66.67	15.00
261	HOH	OH2	-33.68	-20.47	70.17	15.00
262	HOH	OH2	-13.42	-23.06	78.55	15.00
263	HOH	OH2	-8.54	-20.70	73.58	15.00
264	HOH	OH2	-8.22	-29.32	76.42	15.00
265	HOH	OH2	-25.08	-33.76	60.84	15.00
266	HOH	OH2	-23.92	-37.99	66.66	15.00
267	HOH	OH2	-14.04	-33.08	66.81	15.00
268	HOH	OH2	-12.79	-27.03	71.88	15.00
269	HOH	OH2	-18.55	-42.19	77.34	15.00
270	HOH	OH2	-22.19	-37.43	71.34	15.00
271	HOH	OH2	-3.79	-11.43	71.45	15.00
272	HOH	OH2	-10.91	-19.86	67.02	15.00
273	HOH	OH2	-30.22	-20.12	49.07	15.00
274	HOH	OH2	-25.88	-18.93	42.52	15.00
275	HOH	OH2	-36.21	-36.23	51.70	15.00
276	HOH	OH2	-20.20	-20.55	47.99	15.00
277	HOH	OH2	-38.35	-31.19	41.44	15.00
278	HOH	OH2	-37.29	-30.41	51.12	15.00

Table of the orthogonal three dimensional coordinates in Angstroms and B factors (\AA^2) for the cathepsin K complex with inhibitor 1-N-(N-imidazole acetyl-leuciny)-amino-3-N-(4-phenoxy-phenyl-sulfonyl)-amino-propan-2-one.

Residue Atom	X	Y	Z	B
1 ALA CB	-8.26	15.35	87.29	15.00
1 ALA C	-6.43	14.73	88.90	15.00
1 ALA O	-6.17	15.27	89.97	15.00
1 ALA N	-8.92	14.74	89.58	15.00
1 ALA CA	-7.91	14.50	88.49	15.00
2 PRO N	-5.47	14.25	88.09	15.00
2 PRO CD	-5.62	13.29	86.98	15.00
2 PRO CA	-4.05	14.45	88.44	15.00
2 PRO CB	-3.32	13.49	87.50	15.00
2 PRO CG	-4.27	13.38	86.30	15.00
2 PRO C	-3.55	15.87	88.27	15.00
2 PRO O	-4.33	16.79	88.21	15.00
3 ASP N	-2.23	16.02	88.20	15.00
3 ASP CA	-1.59	17.30	88.03	15.00
3 ASP CB	-0.07	17.14	88.15	15.00
3 ASP CG	0.45	17.62	89.50	15.00
3 ASP OD1	-0.04	17.07	90.52	15.00
3 ASP OD2	1.29	18.57	89.55	15.00
3 ASP C	-1.90	18.00	86.73	15.00
3 ASP O	-1.71	17.44	85.64	15.00
4 SER N	-2.32	19.26	86.85	15.00
4 SER CA	-2.67	20.16	85.75	15.00
4 SER CB	-3.63	19.49	84.75	15.00
4 SER OG	-4.80	19.03	85.40	15.00
4 SER C	-3.32	21.45	86.30	15.00
4 SER O	-3.83	21.46	87.42	15.00
5 VAL N	-3.30	22.53	85.53	15.00
5 VAL CA	-3.93	23.80	85.94	15.00
5 VAL CB	-3.00	24.65	86.90	15.00
5 VAL CG1	-1.73	25.13	86.17	15.00
5 VAL CG2	-3.76	25.89	87.45	15.00
5 VAL C	-4.21	24.62	84.69	15.00
5 VAL O	-3.43	24.58	83.75	15.00
6 ASP N	-5.38	25.23	84.60	15.00

6 ASP CA	-5.68	26.09	83.46	15.00
6 ASP CB	-6.83	25.51	82.64	15.00
6 ASP CG	-7.00	26.20	81.28	15.00
6 ASP OD1	-6.01	26.77	80.80	15.00
6 ASP OD2	-8.12	26.17	80.72	15.00
6 ASP C	-6.08	27.42	84.03	15.00
6 ASP O	-7.06	27.49	84.72	15.00
7 TYR N	-5.27	28.45	83.88	15.00
7 TYR CA	-5.62	29.77	84.41	15.00
7 TYR CB	-4.36	30.64	84.56	15.00
7 TYR CG	-3.46	30.18	85.71	15.00
7 TYR CD1	-3.91	30.31	87.05	15.00
7 TYR CE1	-3.20	29.78	88.07	15.00
7 TYR CD2	-2.23	29.50	85.46	15.00
7 TYR CE2	-1.52	28.98	86.45	15.00
7 TYR CZ	-2.00	29.10	87.79	15.00
7 TYR OH	-1.35	28.46	88.84	15.00
7 TYR C	-6.71	30.50	83.66	15.00
7 TYR O	-7.24	31.48	84.14	15.00
8 ARG N	-7.05	29.98	82.49	15.00
8 ARG CA	-8.10	30.59	81.68	15.00
8 ARG CB	-8.09	30.02	80.26	15.00
8 ARG CG	-6.79	30.28	79.56	15.00
8 ARG CD	-6.68	29.59	78.25	15.00
8 ARG NE	-6.70	28.13	78.38	15.00
8 ARG CZ	-6.78	27.29	77.36	15.00
8 ARG NH1	-6.85	27.73	76.13	15.00
8 ARG NH2	-6.72	25.99	77.58	15.00
8 ARG C	-9.44	30.40	82.35	15.00
8 ARG O	-10.24	31.34	82.45	15.00
9 LYS N	-9.68	29.21	82.87	15.00
9 LYS CA	-10.94	28.95	83.54	15.00
9 LYS CB	-11.17	27.45	83.73	15.00
9 LYS CG	-11.06	26.59	82.48	15.00
9 LYS CD	-11.19	25.12	82.85	15.00
9 LYS CE	-11.10	24.18	81.67	15.00
9 LYS NZ	-11.53	22.81	82.08	15.00
9 LYS C	-10.96	29.61	84.91	15.00
9 LYS O	-12.02	29.58	85.59	15.00
10 LYS N	-9.86	30.26	85.31	15.00
10 LYS CA	-9.84	30.86	86.64	15.00
10 LYS CB	-8.57	30.42	87.38	15.00
10 LYS CG	-8.45	28.89	87.51	15.00

TABLE X

10	LYS	CD	-7.03	28.46	87.81	15.00
10	LYS	CE	-6.43	29.14	89.04	15.00
10	LYS	NZ	-7.24	28.91	90.30	15.00
10	LYS	C	-9.98	32.40	86.61	15.00
10	LYS	O	-10.16	33.04	87.64	15.00
11	GLY	N	-9.85	32.98	85.41	15.00
11	GLY	CA	-9.94	34.41	85.22	15.00
11	GLY	C	-8.63	35.17	85.27	15.00
11	GLY	O	-8.61	36.39	85.26	15.00
12	TYR	N	-7.54	34.42	85.20	15.00
12	TYR	CA	-6.21	34.98	85.26	15.00
12	TYR	CB	-5.24	33.95	85.84	15.00
12	TYR	CG	-5.32	33.72	87.35	15.00
12	TYR	CD1	-6.52	33.50	87.99	15.00
12	TYR	CE1	-6.58	33.26	89.37	15.00
12	TYR	CD2	-4.18	33.66	88.13	15.00
12	TYR	CE2	-4.23	33.42	89.47	15.00
12	TYR	CZ	-5.42	33.23	90.06	15.00
12	TYR	OH	-5.43	33.02	91.43	15.00
12	TYR	C	-5.68	35.43	83.90	15.00
12	TYR	O	-4.68	36.17	83.83	15.00
13	VAL	N	-6.34	35.06	82.81	15.00
13	VAL	CA	-5.82	35.45	81.50	15.00
13	VAL	CB	-5.54	34.18	80.66	15.00
13	VAL	CG1	-4.93	34.52	79.31	15.00
13	VAL	CG2	-4.58	33.24	81.42	15.00
13	VAL	C	-6.76	36.37	80.72	15.00
13	VAL	O	-7.95	36.17	80.78	15.00
14	THR	N	-6.24	37.41	80.08	15.00
14	THR	CA	-7.06	38.29	79.27	15.00
14	THR	CB	-6.41	39.67	79.12	15.00
14	THR	OG1	-5.06	39.53	78.69	15.00
14	THR	CG2	-6.48	40.43	80.39	15.00
14	THR	C	-7.20	37.68	77.89	15.00
14	THR	O	-6.41	36.81	77.48	15.00
15	PRO	N	-8.14	38.18	77.09	15.00
15	PRO	CD	-9.11	39.26	77.34	15.00
15	PRO	CA	-8.33	37.64	75.75	15.00
15	PRO	CB	-9.51	38.47	75.23	15.00
15	PRO	CG	-9.35	39.77	75.97	15.00
15	PRO	C	-7.09	37.85	74.89	15.00
15	PRO	O	-6.26	38.73	75.17	15.00
16	VAL	N	-6.96	37.00	73.87	15.00

TABLE X

16 VAL CA	-5.81	37.05	73.00	15.00
16 VAL CB	-5.74	35.80	72.11	15.00
16 VAL CG1	-4.42	35.77	71.35	15.00
16 VAL CG2	-5.84	34.56	72.97	15.00
16 VAL C	-5.76	38.30	72.12	15.00
16 VAL O	-6.70	38.61	71.37	15.00
17 LYS N	-4.58	38.91	72.12	15.00
17 LYS CA	-4.36	40.08	71.32	15.00
17 LYS CB	-3.75	41.20	72.15	15.00
17 LYS CG	-4.73	42.01	72.95	15.00
17 LYS CD	-5.27	41.23	74.12	15.00
17 LYS CE	-5.71	42.11	75.23	15.00
17 LYS NZ	-5.93	41.40	76.53	15.00
17 LYS C	-3.45	39.72	70.16	15.00
17 LYS O	-2.83	38.63	70.16	15.00
18 ASN N	-3.32	40.68	69.24	15.00
18 ASN CA	-2.51	40.54	68.03	15.00
18 ASN CB	-3.37	40.84	66.84	15.00
18 ASN CG	-2.76	40.33	65.56	15.00
18 ASN OD1	-1.57	40.56	65.29	15.00
18 ASN ND2	-3.55	39.60	64.78	15.00
18 ASN C	-1.33	41.51	68.00	15.00
18 ASN O	-1.50	42.73	67.86	15.00
19 GLN N	-0.15	40.93	68.03	15.00
19 GLN CA	1.12	41.67	68.01	15.00
19 GLN CB	2.23	40.66	67.93	15.00
19 GLN CG	3.64	41.21	67.96	15.00
19 GLN CD	4.65	40.13	68.03	15.00
19 GLN OE1	4.35	39.00	68.42	15.00
19 GLN NE2	5.86	40.47	67.64	15.00
19 GLN C	1.22	42.69	66.88	15.00
19 GLN O	1.75	43.75	67.04	15.00
20 GLY N	0.66	42.38	65.74	15.00
20 GLY CA	0.66	43.27	64.59	15.00
20 GLY C	1.84	42.90	63.73	15.00
20 GLY O	1.98	41.74	63.33	15.00
21 GLN N	2.67	43.89	63.43	15.00
21 GLN CA	3.88	43.70	62.61	15.00
21 GLN CB	3.90	44.62	61.39	15.00
21 GLN CG	2.90	44.23	60.27	15.00
21 GLN CD	3.33	43.03	59.44	15.00
21 GLN OE1	4.25	43.10	58.59	15.00
21 GLN NE2	2.58	41.95	59.58	15.00

TABLE X

21 GLN C	5.05	44.09	63.52	15.00
21 GLN O	6.20	43.88	63.19	15.00
22 CYS N	4.74	44.77	64.60	15.00
22 CYS CA	5.74	45.22	65.53	15.00
22 CYS C	6.26	44.01	66.35	15.00
22 CYS O	5.48	43.07	66.60	15.00
22 CYS CB	5.08	46.25	66.43	15.00
22 CYS SG	6.07	46.62	67.91	15.00
23 GLY N	7.57	43.99	66.68	15.00
23 GLY CA	8.16	42.91	67.47	15.00
23 GLY C	8.07	43.16	68.96	15.00
23 GLY O	9.08	43.15	69.68	15.00
24 SER N	6.82	43.29	69.42	15.00
24 SER CA	6.47	43.55	70.79	15.00
24 SER CB	5.45	44.66	70.86	15.00
24 SER OG	4.31	44.30	70.15	15.00
24 SER C	5.97	42.28	71.46	15.00
24 SER O	5.26	42.34	72.45	15.00
25 CYS N	6.43	41.13	70.98	15.00
25 CYS CA	6.06	39.87	71.53	15.00
25 CYS CB	6.61	38.78	70.65	15.00
25 CYS SG	8.41	38.83	70.46	15.00
25 CYS C	6.49	39.79	73.01	15.00
25 CYS O	5.74	39.28	73.84	15.00
25 INH C1	3.24	39.22	63.40	15.00
25 INH C2	2.86	38.72	62.13	15.00
25 INH C3	1.57	38.27	61.89	15.00
25 INH C4	0.62	38.31	62.90	15.00
25 INH C5	0.94	38.79	64.16	15.00
25 INH C6	2.25	39.24	64.42	15.00
25 INH O7	4.57	39.75	63.63	15.00
25 INH C8	5.72	39.02	63.91	15.00
25 INH C9	5.62	38.42	65.17	15.00
25 INH C10	6.58	37.50	65.60	15.00
25 INH C11	7.65	37.17	64.78	15.00
25 INH C12	7.79	37.78	63.51	15.00
25 INH C13	6.82	38.71	63.08	15.00
25 INH S14	8.67	35.93	65.55	15.00
25 INH O15	7.93	34.70	65.54	15.00
25 INH O16	9.92	35.97	64.82	15.00
25 INH N17	8.95	36.39	67.18	15.00
25 INH C18	9.50	37.70	67.57	15.00
25 INH C19	9.05	38.78	68.64	15.00

TABLE X

25 INH O20	8.53	39.68	67.70	15.00
25 INH C21	10.52	39.34	69.16	15.00
25 INH N22	11.16	38.50	70.20	15.00
25 INH C23	12.14	38.91	71.00	15.00
25 INH O24	12.59	40.07	70.97	15.00
25 INH C25	12.61	37.92	72.07	15.00
25 INH C26	11.69	38.19	73.25	15.00
25 INH C27	11.80	37.33	74.48	15.00
25 INH C28	12.06	35.90	74.03	15.00
25 INH C29	12.95	37.84	75.32	15.00
25 INH N30	14.03	38.09	72.47	15.00
25 INH C31	14.92	37.10	72.44	15.00
25 INH O32	14.63	35.96	72.06	15.00
25 INH C33	16.36	37.38	72.94	15.00
25 INH C34	17.21	36.17	73.26	15.00
25 INH C35	17.54	35.58	74.44	15.00
25 INH N36	18.35	34.51	74.16	15.00
25 INH C37	18.52	34.43	72.85	15.00
25 INH N38	17.85	35.42	72.28	15.00
26 TRP N	7.57	40.50	73.34	15.00
26 TRP CA	8.08	40.58	74.69	15.00
26 TRP CB	9.55	41.06	74.66	15.00
26 TRP CG	9.72	42.45	74.12	15.00
26 TRP CD2	9.74	43.67	74.85	15.00
26 TRP CE2	9.80	44.74	73.89	15.00
26 TRP CE3	9.72	43.99	76.22	15.00
26 TRP CD1	9.78	42.79	72.83	15.00
26 TRP NE1	9.82	44.15	72.67	15.00
26 TRP CZ2	9.83	46.10	74.25	15.00
26 TRP CZ3	9.75	45.31	76.58	15.00
26 TRP CH2	9.81	46.37	75.59	15.00
26 TRP C	7.21	41.51	75.60	15.00
26 TRP O	7.08	41.27	76.81	15.00
27 ALA N	6.58	42.54	75.01	15.00
27 ALA CA	5.77	43.48	75.79	15.00
27 ALA CB	5.51	44.71	74.96	15.00
27 ALA C	4.47	42.75	76.05	15.00
27 ALA O	3.88	42.85	77.12	15.00
28 PHE N	4.07	41.90	75.13	15.00
28 PHE CA	2.81	41.20	75.33	15.00
28 PHE CB	2.29	40.66	73.99	15.00
28 PHE CG	1.55	41.68	73.15	15.00
28 PHE CD1	2.23	42.39	72.20	15.00

TABLE X

28 PHE CD2	0.19	41.92	73.31	15.00
28 PHE CE1	1.57	43.34	71.43	15.00
28 PHE CE2	-0.46	42.87	72.55	15.00
28 PHE CZ	0.23	43.58	71.61	15.00
28 PHE C	2.87	40.12	76.46	15.00
28 PHE O	1.92	39.99	77.26	15.00
29 SER N	3.97	39.39	76.54	15.00
29 SER CA	4.16	38.37	77.55	15.00
29 SER CB	5.40	37.55	77.18	15.00
29 SER OG	5.72	36.66	78.21	15.00
29 SER C	4.28	38.96	78.94	15.00
29 SER O	3.68	38.47	79.91	15.00
30 SER N	5.04	40.05	79.02	15.00
30 SER CA	5.25	40.76	80.28	15.00
30 SER CB	6.13	41.95	80.06	15.00
30 SER OG	7.38	41.52	79.59	15.00
30 SER C	3.96	41.22	80.96	15.00
30 SER O	3.72	40.99	82.17	15.00
31 VAL N	3.13	41.85	80.14	15.00
31 VAL CA	1.83	42.35	80.51	15.00
31 VAL CB	1.33	43.26	79.35	15.00
31 VAL CG1	-0.15	43.27	79.23	15.00
31 VAL CG2	1.86	44.66	79.52	15.00
31 VAL C	0.91	41.16	80.90	15.00
31 VAL O	0.02	41.32	81.77	15.00
32 GLY N	1.16	39.98	80.31	15.00
32 GLY CA	0.35	38.81	80.61	15.00
32 GLY C	0.70	38.25	81.97	15.00
32 GLY O	-0.17	37.79	82.70	15.00
33 ALA N	1.98	38.30	82.34	15.00
33 ALA CA	2.47	37.84	83.63	15.00
33 ALA CB	3.98	37.93	83.67	15.00
33 ALA C	1.84	38.86	84.60	15.00
33 ALA O	1.09	38.48	85.52	15.00
34 LEU N	2.09	40.15	84.37	15.00
34 LEU CA	1.54	41.22	85.20	15.00
34 LEU CB	1.88	42.56	84.56	15.00
34 LEU CG	3.30	43.17	84.66	15.00
34 LEU CD1	3.26	44.56	84.13	15.00
34 LEU CD2	3.76	43.24	86.11	15.00
34 LEU C	0.02	41.13	85.45	15.00
34 LEU O	-0.47	41.28	86.60	15.00
35 GLU N	-0.70	40.80	84.39	15.00

TABLE X

35 GLU CA	-2.16	40.62	84.49	15.00
35 GLU CB	-2.77	40.37	83.11	15.00
35 GLU CG	-2.92	41.61	82.27	15.00
35 GLU CD	-3.06	41.33	80.78	15.00
35 GLU OE1	-2.97	40.14	80.38	15.00
35 GLU OE2	-3.31	42.29	80.00	15.00
35 GLU C	-2.60	39.51	85.47	15.00
35 GLU O	-3.31	39.78	86.45	15.00
36 GLY N	-2.11	38.29	85.24	15.00
36 GLY CA	-2.42	37.14	86.06	15.00
36 GLY C	-2.20	37.38	87.56	15.00
36 GLY O	-2.96	36.89	88.40	15.00
37 GLN N	-1.13	38.09	87.89	15.00
37 GLN CA	-0.78	38.39	89.27	15.00
37 GLN CB	0.64	38.96	89.35	15.00
37 GLN CG	1.72	37.92	89.12	15.00
37 GLN CD	1.50	36.73	90.00	15.00
37 GLN OE1	1.69	36.81	91.20	15.00
37 GLN NE2	1.12	35.61	89.42	15.00
37 GLN C	-1.78	39.38	89.83	15.00
37 GLN O	-2.30	39.19	90.94	15.00
38 LEU N	-2.10	40.38	89.02	15.00
38 LEU CA	-3.04	41.41	89.38	15.00
38 LEU CB	-3.28	42.29	88.15	15.00
38 LEU CG	-4.10	43.56	88.33	15.00
38 LEU CD1	-3.72	44.25	89.66	15.00
38 LEU CD2	-3.95	44.48	87.16	15.00
38 LEU C	-4.32	40.75	89.82	15.00
38 LEU O	-4.90	41.05	90.86	15.00
39 LYS N	-4.75	39.78	89.04	15.00
39 LYS CA	-5.95	39.07	89.36	15.00
39 LYS CB	-6.29	38.15	88.20	15.00
39 LYS CG	-7.34	37.13	88.56	15.00
39 LYS CD	-8.65	37.80	88.80	15.00
39 LYS CE	-9.71	36.74	88.86	15.00
39 LYS NZ	-10.82	37.33	89.61	15.00
39 LYS C	-5.78	38.28	90.67	15.00
39 LYS O	-6.62	38.34	91.53	15.00
40 LYS N	-4.66	37.59	90.83	15.00
40 LYS CA	-4.40	36.83	92.03	15.00
40 LYS CB	-3.01	36.20	91.96	15.00
40 LYS CG	-2.68	35.31	93.16	15.00
40 LYS CD	-1.38	34.53	93.00	15.00

TABLE X

40 LYS CE	-1.10	33.63	94.23	15.00
40 LYS NZ	-0.27	32.41	93.89	15.00
40 LYS C	-4.50	37.71	93.27	15.00
40 LYS O	-5.26	37.42	94.20	15.00
41 LYS N	-3.86	38.87	93.18	15.00
41 LYS CA	-3.77	39.84	94.28	15.00
41 LYS CB	-2.31	40.32	94.41	15.00
41 LYS CG	-1.28	39.21	94.20	15.00
41 LYS CD	-0.04	39.35	95.07	15.00
41 LYS CE	0.68	38.01	95.15	15.00
41 LYS NZ	-0.14	36.86	95.66	15.00
41 LYS C	-4.64	41.07	94.09	15.00
41 LYS O	-4.15	42.18	94.26	15.00
42 THR N	-5.91	40.88	93.78	15.00
42 THR CA	-6.80	42.01	93.60	15.00
42 THR CB	-6.50	42.75	92.28	15.00
42 THR OG1	-5.17	43.26	92.28	15.00
42 THR CG2	-7.48	43.85	92.07	15.00
42 THR C	-8.22	41.47	93.50	15.00
42 THR O	-9.17	42.02	94.07	15.00
43 GLY N	-8.37	40.40	92.74	15.00
43 GLY CA	-9.67	39.80	92.56	15.00
43 GLY C	-10.28	40.20	91.22	15.00
43 GLY O	-11.22	39.57	90.74	15.00
44 LYS N	-9.65	41.19	90.58	15.00
44 LYS CA	-10.13	41.70	89.32	15.00
44 LYS CB	-10.71	43.10	89.52	15.00
44 LYS CG	-11.95	43.16	90.39	15.00
44 LYS CD	-12.36	44.57	90.76	15.00
44 LYS CE	-11.43	45.21	91.78	15.00
44 LYS NZ	-11.50	44.47	93.08	15.00
44 LYS C	-9.02	41.76	88.30	15.00
44 LYS O	-7.91	42.20	88.61	15.00
45 LEU N	-9.35	41.40	87.07	15.00
45 LEU CA	-8.38	41.39	85.99	15.00
45 LEU CB	-8.61	40.14	85.13	15.00
45 LEU CG	-7.85	39.77	83.85	15.00
45 LEU CD1	-6.47	39.23	84.16	15.00
45 LEU CD2	-8.67	38.72	83.14	15.00
45 LEU C	-8.55	42.68	85.16	15.00
45 LEU O	-9.55	43.36	85.27	15.00
46 LEU N	-7.57	43.04	84.37	15.00
46 LEU CA	-7.65	44.23	83.55	15.00

TABLE X

46 LEU CB	-7.27	45.46	84.35	15.00
46 LEU CG	-7.82	46.76	83.83	15.00
46 LEU CD1	-9.28	46.67	83.92	15.00
46 LEU CD2	-7.33	47.91	84.71	15.00
46 LEU C	-6.63	44.03	82.45	15.00
46 LEU O	-5.67	43.30	82.61	15.00
47 ASN N	-6.80	44.76	81.36	15.00
47 ASN CA	-5.90	44.66	80.25	15.00
47 ASN CB	-6.61	45.08	78.95	15.00
47 ASN CG	-7.47	43.98	78.39	15.00
47 ASN OD1	-7.52	42.88	78.93	15.00
47 ASN ND2	-8.19	44.28	77.33	15.00
47 ASN C	-4.77	45.63	80.52	15.00
47 ASN O	-5.02	46.82	80.64	15.00
48 LEU N	-3.54	45.17	80.66	15.00
48 LEU CA	-2.44	46.13	80.87	15.00
48 LEU CB	-1.29	45.54	81.75	15.00
48 LEU CG	-1.76	45.23	83.19	15.00
48 LEU CD1	-0.62	44.99	84.10	15.00
48 LEU CD2	-2.69	46.29	83.75	15.00
48 LEU C	-1.96	46.66	79.51	15.00
48 LEU O	-2.40	46.14	78.46	15.00
49 SER N	-1.12	47.70	79.52	15.00
49 SER CA	-0.63	48.29	78.28	15.00
49 SER CB	-0.70	49.82	78.41	15.00
49 SER OG	0.06	50.46	77.43	15.00
49 SER C	0.75	47.87	77.84	15.00
49 SER O	1.75	48.29	78.43	15.00
50 PRO N	0.81	47.08	76.75	15.00
50 PRO CD	-0.34	46.48	76.03	15.00
50 PRO CA	2.10	46.61	76.22	15.00
50 PRO CB	1.68	45.45	75.34	15.00
50 PRO CG	0.33	45.96	74.79	15.00
50 PRO C	2.77	47.79	75.45	15.00
50 PRO O	3.99	47.96	75.47	15.00
51 GLN N	1.96	48.67	74.86	15.00
51 GLN CA	2.48	49.87	74.18	15.00
51 GLN CB	1.37	50.77	73.66	15.00
51 GLN CG	2.00	51.92	72.85	15.00
51 GLN CD	2.33	51.51	71.46	15.00
51 GLN OE1	1.83	50.49	70.97	15.00
51 GLN NE2	3.19	52.26	70.81	15.00
51 GLN C	3.29	50.70	75.17	15.00

TABLE X

51 GLN O	4.21	51.38	74.79	15.00
52 ASN N	2.93	50.65	76.45	15.00
52 ASN CA	3.62	51.40	77.47	15.00
52 ASN CB	2.96	51.15	78.82	15.00
52 ASN CG	3.52	52.04	79.91	15.00
52 ASN OD1	4.31	52.93	79.64	15.00
52 ASN ND2	3.09	51.81	81.14	15.00
52 ASN C	5.04	50.91	77.52	15.00
52 ASN O	5.98	51.71	77.54	15.00
53 LEU N	5.19	49.60	77.57	15.00
53 LEU CA	6.53	49.05	77.64	15.00
53 LEU CB	6.40	47.59	77.98	15.00
53 LEU CG	5.80	47.51	79.34	15.00
53 LEU CD1	5.66	46.07	79.79	15.00
53 LEU CD2	6.65	48.34	80.33	15.00
53 LEU C	7.25	49.26	76.30	15.00
53 LEU O	8.43	49.52	76.27	15.00
54 VAL N	6.53	49.17	75.19	15.00
54 VAL CA	7.19	49.34	73.89	15.00
54 VAL CB	6.25	49.16	72.69	15.00
54 VAL CG1	6.98	49.50	71.41	15.00
54 VAL CG2	5.83	47.75	72.63	15.00
54 VAL C	7.89	50.66	73.74	15.00
54 VAL O	9.06	50.71	73.32	15.00
55 ASP N	7.28	51.70	74.27	15.00
55 ASP CA	7.87	53.05	74.15	15.00
55 ASP CB	6.76	54.08	73.93	15.00
55 ASP CG	5.70	53.58	72.94	15.00
55 ASP OD1	5.95	52.76	72.00	15.00
55 ASP OD2	4.60	54.09	73.02	15.00
55 ASP C	8.68	53.42	75.33	15.00
55 ASP O	9.58	54.23	75.23	15.00
56 CYS N	8.38	52.90	76.50	15.00
56 CYS CA	9.13	53.37	77.67	15.00
56 CYS C	10.33	52.59	78.21	15.00
56 CYS O	11.25	53.15	78.82	15.00
56 CYS CB	8.16	53.80	78.81	15.00
56 CYS SG	6.73	54.73	78.24	15.00
57 VAL N	10.39	51.31	77.97	15.00
57 VAL CA	11.49	50.47	78.46	15.00
57 VAL CB	11.10	48.99	78.38	15.00
57 VAL CG1	12.15	48.16	78.95	15.00
57 VAL CG2	9.83	48.77	79.11	15.00

TABLE X

57 VAL C	12.66	50.67	77.55	15.00
57 VAL O	12.94	49.87	76.66	15.00
58 SER N	13.40	51.73	77.79	15.00
58 SER CA	14.54	52.04	76.91	15.00
58 SER CB	15.13	53.44	77.26	15.00
58 SER OG	15.02	53.68	78.65	15.00
58 SER C	15.61	50.98	76.86	15.00
58 SER O	16.39	50.92	75.91	15.00
59 GLU N	15.66	50.15	77.91	15.00
59 GLU CA	16.66	49.07	78.00	15.00
59 GLU CB	16.59	48.34	79.35	15.00
59 GLU CG	16.98	49.19	80.58	15.00
59 GLU CD	15.98	50.33	80.88	15.00
59 GLU OE1	14.75	50.10	80.81	15.00
59 GLU OE2	16.46	51.46	81.17	15.00
59 GLU C	16.48	48.04	76.89	15.00
59 GLU O	17.36	47.20	76.67	15.00
60 ASN N	15.31	48.07	76.27	15.00
60 ASN CA	15.00	47.16	75.19	15.00
60 ASN CB	13.64	46.51	75.47	15.00
60 ASN CG	13.69	45.49	76.59	15.00
60 ASN OD1	12.76	45.39	77.36	15.00
60 ASN ND2	14.76	44.68	76.63	15.00
60 ASN C	14.98	47.89	73.85	15.00
60 ASN O	15.26	49.09	73.79	15.00
61 ASP N	14.67	47.16	72.79	15.00
61 ASP CA	14.64	47.72	71.44	15.00
61 ASP CB	15.38	46.80	70.48	15.00
61 ASP CG	16.10	47.57	69.36	15.00
61 ASP OD1	16.04	48.81	69.34	15.00
61 ASP OD2	16.76	46.92	68.52	15.00
61 ASP C	13.28	48.07	70.81	15.00
61 ASP O	13.13	48.13	69.60	15.00
62 GLY N	12.31	48.40	71.63	15.00
62 GLY CA	10.98	48.67	71.11	15.00
62 GLY C	10.49	47.51	70.24	15.00
62 GLY O	10.64	46.38	70.57	15.00
63 CYS N	9.98	47.80	69.05	15.00
63 CYS CA	9.47	46.79	68.11	15.00
63 CYS C	10.61	45.95	67.62	15.00
63 CYS O	10.41	45.05	66.81	15.00
63 CYS CB	8.71	47.45	66.95	15.00
63 CYS SG	7.16	48.19	67.39	15.00

TABLE X

64 GLY N	11.82	46.25	68.06	15.00
64 GLY CA	12.94	45.47	67.59	15.00
64 GLY C	13.32	44.36	68.55	15.00
64 GLY O	14.37	43.74	68.40	15.00
65 GLY N	12.48	44.12	69.55	15.00
65 GLY CA	12.76	43.06	70.49	15.00
65 GLY C	13.11	43.58	71.88	15.00
65 GLY O	13.33	44.80	72.13	15.00
66 GLY N	13.21	42.63	72.80	15.00
66 GLY CA	13.50	43.00	74.18	15.00
66 GLY C	13.34	41.82	75.15	15.00
66 GLY O	12.91	40.73	74.72	15.00
67 TYR N	13.65	42.02	76.42	15.00
67 TYR CA	13.55	40.94	77.37	15.00
67 TYR CB	14.85	40.83	78.19	15.00
67 TYR CG	16.13	40.41	77.42	15.00
67 TYR CD1	16.31	39.16	76.96	15.00
67 TYR CE1	17.51	38.78	76.29	15.00
67 TYR CD2	17.13	41.25	77.20	15.00
67 TYR CE2	18.32	40.83	76.53	15.00
67 TYR CZ	18.49	39.61	76.08	15.00
67 TYR OH	19.63	39.12	75.47	15.00
67 TYR C	12.41	41.24	78.31	15.00
67 TYR O	12.00	42.40	78.46	15.00
68 MET N	11.84	40.20	78.88	15.00
68 MET CA	10.72	40.40	79.78	15.00
68 MET CB	10.01	39.09	80.00	15.00
68 MET CG	9.14	38.63	78.85	15.00
68 MET SD	10.15	37.92	77.61	15.00
68 MET CE	10.37	36.10	78.19	15.00
68 MET C	11.20	41.05	81.10	15.00
68 MET O	10.55	41.92	81.68	15.00
69 THR N	12.33	40.56	81.59	15.00
69 THR CA	12.91	41.02	82.85	15.00
69 THR CB	14.24	40.26	83.21	15.00
69 THR OG1	15.16	40.38	82.12	15.00
69 THR CG2	13.99	38.77	83.56	15.00
69 THR C	13.15	42.55	82.80	15.00
69 THR O	13.15	43.20	83.83	15.00
70 ASN N	13.42	43.10	81.63	15.00
70 ASN CA	13.61	44.55	81.51	15.00
70 ASN CB	14.23	44.95	80.15	15.00
70 ASN CG	15.73	44.64	80.08	15.00

TABLE X

70 ASN OD1	16.28	44.44	78.98	15.00
70 ASN ND2	16.41	44.61	81.22	15.00
70 ASN C	12.27	45.27	81.66	15.00
70 ASN O	12.24	46.42	82.08	15.00
71 ALA N	11.20	44.62	81.19	15.00
71 ALA CA	9.84	45.13	81.24	15.00
71 ALA CB	8.96	44.17	80.50	15.00
71 ALA C	9.39	45.23	82.69	15.00
71 ALA O	8.79	46.23	83.13	15.00
72 PHE N	9.72	44.17	83.43	15.00
72 PHE CA	9.39	44.09	84.87	15.00
72 PHE CB	9.67	42.66	85.39	15.00
72 PHE CG	8.80	41.59	84.75	15.00
72 PHE CD1	7.52	41.87	84.33	15.00
72 PHE CD2	9.28	40.32	84.57	15.00
72 PHE CE1	6.73	40.91	83.73	15.00
72 PHE CE2	8.50	39.35	83.98	15.00
72 PHE CZ	7.23	39.64	83.56	15.00
72 PHE C	10.19	45.09	85.71	15.00
72 PHE O	9.73	45.60	86.72	15.00
73 GLN N	11.41	45.38	85.28	15.00
73 GLN CA	12.27	46.36	85.97	15.00
73 GLN CB	13.74	46.30	85.47	15.00
73 GLN CG	14.74	46.94	86.38	15.00
73 GLN CD	14.58	46.42	87.78	15.00
73 GLN OE1	14.18	45.26	87.96	15.00
73 GLN NE2	14.76	47.28	88.79	15.00
73 GLN C	11.74	47.79	85.84	15.00
73 GLN O	11.83	48.57	86.78	15.00
74 TYR N	11.23	48.14	84.67	15.00
74 TYR CA	10.67	49.45	84.41	15.00
74 TYR CB	10.48	49.62	82.93	15.00
74 TYR CG	9.52	50.72	82.59	15.00
74 TYR CD1	9.90	51.97	82.44	15.00
74 TYR CE1	8.98	53.00	82.06	15.00
74 TYR CD2	8.25	50.50	82.38	15.00
74 TYR CE2	7.39	51.55	82.01	15.00
74 TYR CZ	7.74	52.77	81.85	15.00
74 TYR OH	6.87	53.67	81.39	15.00
74 TYR C	9.35	49.64	85.16	15.00
74 TYR O	9.04	50.74	85.58	15.00
75 VAL N	8.60	48.58	85.39	15.00
75 VAL CA	7.35	48.70	86.13	15.00

TABLE X

75 VAL CB	6.46	47.47	85.92	15.00
75 VAL CG1	5.15	47.64	86.74	15.00
75 VAL CG2	6.10	47.32	84.44	15.00
75 VAL C	7.63	48.95	87.62	15.00
75 VAL O	6.92	49.76	88.26	15.00
76 GLN N	8.69	48.31	88.13	15.00
76 GLN CA	9.12	48.47	89.51	15.00
76 GLN CB	10.10	47.35	89.89	15.00
76 GLN CG	10.55	47.31	91.38	15.00
76 GLN CD	11.76	46.41	91.65	15.00
76 GLN OE1	12.14	46.22	92.80	15.00
76 GLN NE2	12.37	45.85	90.59	15.00
76 GLN C	9.78	49.88	89.59	15.00
76 GLN O	9.37	50.72	90.39	15.00
77 LYS N	10.72	50.19	88.69	15.00
77 LYS CA	11.40	51.49	88.72	15.00
77 LYS CB	12.56	51.50	87.72	15.00
77 LYS CG	13.20	52.85	87.44	15.00
77 LYS CD	14.22	52.70	86.33	15.00
77 LYS CE	15.18	51.56	86.62	15.00
77 LYS NZ	16.20	51.34	85.56	15.00
77 LYS C	10.51	52.71	88.55	15.00
77 LYS O	10.73	53.76	89.17	15.00
78 ASN N	9.50	52.55	87.70	15.00
78 ASN CA	8.51	53.59	87.37	15.00
78 ASN CB	7.84	53.25	86.04	15.00
78 ASN CG	7.15	54.42	85.42	15.00
78 ASN OD1	7.70	55.49	85.36	15.00
78 ASN ND2	5.93	54.22	84.95	15.00
78 ASN C	7.44	53.69	88.42	15.00
78 ASN O	6.89	54.77	88.64	15.00
79 ARG N	7.15	52.56	89.05	15.00
79 ARG CA	6.14	52.48	90.08	15.00
79 ARG CB	6.27	53.65	91.07	15.00
79 ARG CG	7.58	53.69	91.85	15.00
79 ARG CD	7.76	55.00	92.63	15.00
79 ARG NE	6.66	55.34	93.55	15.00
79 ARG CZ	6.30	54.65	94.63	15.00
79 ARG NH1	6.95	53.54	94.96	15.00
79 ARG NH2	5.21	55.01	95.31	15.00
79 ARG C	4.77	52.46	89.43	15.00
79 ARG O	3.80	52.99	90.00	15.00
80 GLY N	4.66	51.78	88.30	15.00

TABLE X

80 GLY CA	3.39	51.70	87.64	15.00
80 GLY C	3.39	51.50	86.16	15.00
80 GLY O	4.32	51.90	85.43	15.00
81 ILE N	2.30	50.87	85.73	15.00
81 ILE CA	2.03	50.55	84.34	15.00
81 ILE CB	2.38	49.06	83.98	15.00
81 ILE CG2	1.41	48.10	84.64	15.00
81 ILE CG1	2.48	48.88	82.46	15.00
81 ILE CD1	2.67	47.47	82.00	15.00
81 ILE C	0.57	50.92	84.01	15.00
81 ILE O	-0.33	50.73	84.82	15.00
82 ASP N	0.35	51.53	82.85	15.00
82 ASP CA	-1.01	51.93	82.43	15.00
82 ASP CB	-0.91	52.93	81.27	15.00
82 ASP CG	-0.45	54.32	81.71	15.00
82 ASP OD1	0.52	54.88	81.14	15.00
82 ASP OD2	-1.08	54.84	82.64	15.00
82 ASP C	-1.87	50.76	82.00	15.00
82 ASP O	-1.39	49.64	81.87	15.00
83 SER N	-3.16	51.03	81.87	15.00
83 SER CA	-4.11	50.02	81.42	15.00
83 SER CB	-5.54	50.23	82.00	15.00
83 SER OG	-5.97	51.58	81.87	15.00
83 SER C	-4.14	50.20	79.91	15.00
83 SER O	-3.48	51.11	79.34	15.00
84 GLU N	-4.79	49.26	79.24	15.00
84 GLU CA	-4.92	49.33	77.79	15.00
84 GLU CB	-5.77	48.16	77.25	15.00
84 GLU CG	-5.57	47.95	75.77	15.00
84 GLU CD	-4.09	47.91	75.42	15.00
84 GLU OE1	-3.52	48.88	74.89	15.00
84 GLU OE2	-3.46	46.90	75.73	15.00
84 GLU C	-5.65	50.62	77.45	15.00
84 GLU O	-5.13	51.48	76.76	15.00
85 ASP N	-6.84	50.77	78.03	15.00
85 ASP CA	-7.68	51.96	77.78	15.00
85 ASP CB	-9.03	51.85	78.51	15.00
85 ASP CG	-9.94	53.12	78.30	15.00
85 ASP OD1	-10.32	53.78	79.30	15.00
85 ASP OD2	-10.26	53.46	77.15	15.00
85 ASP C	-7.01	53.27	78.08	15.00
85 ASP O	-7.29	54.29	77.43	15.00
86 ALA N	-6.11	53.26	79.05	15.00

TABLE X

86	ALA	CA	-5.41	54.47	79.38	15.00
86	ALA	CB	-4.88	54.38	80.80	15.00
86	ALA	C	-4.27	54.73	78.39	15.00
86	ALA	O	-4.00	55.89	78.07	15.00
87	TYR	N	-3.69	53.66	77.83	15.00
87	TYR	CA	-2.57	53.78	76.88	15.00
87	TYR	CB	-1.24	53.68	77.66	15.00
87	TYR	CG	0.04	54.14	77.00	15.00
87	TYR	CD1	0.10	54.44	75.56	15.00
87	TYR	CE1	1.32	54.83	74.98	15.00
87	TYR	CD2	1.21	54.26	77.84	15.00
87	TYR	CE2	2.42	54.65	77.33	15.00
87	TYR	CZ	2.49	54.94	75.86	15.00
87	TYR	OH	3.71	55.29	75.29	15.00
87	TYR	C	-2.68	52.66	75.83	15.00
87	TYR	O	-2.00	51.63	75.92	15.00
88	PRO	N	-3.51	52.90	74.79	15.00
88	PRO	CD	-4.53	53.97	74.75	15.00
88	PRO	CA	-3.75	51.94	73.71	15.00
88	PRO	CB	-4.87	52.62	72.90	15.00
88	PRO	CG	-5.64	53.31	73.98	15.00
88	PRO	C	-2.52	51.62	72.84	15.00
88	PRO	O	-1.59	52.42	72.70	15.00
89	TYR	N	-2.58	50.42	72.24	15.00
89	TYR	CA	-1.54	49.87	71.38	15.00
89	TYR	CB	-1.64	48.34	71.47	15.00
89	TYR	CG	-0.54	47.59	70.84	15.00
89	TYR	CD1	0.79	47.78	71.31	15.00
89	TYR	CE1	1.83	47.13	70.72	15.00
89	TYR	CD2	-0.80	46.69	69.76	15.00
89	TYR	CE2	0.20	46.03	69.15	15.00
89	TYR	CZ	1.53	46.24	69.61	15.00
89	TYR	OH	2.55	45.63	68.93	15.00
89	TYR	C	-1.73	50.30	69.92	15.00
89	TYR	O	-2.81	50.16	69.38	15.00
90	VAL	N	-0.65	50.73	69.28	15.00
90	VAL	CA	-0.69	51.22	67.88	15.00
90	VAL	CB	-0.15	52.67	67.77	15.00
90	VAL	CG1	-0.81	53.58	68.80	15.00
90	VAL	CG2	1.34	52.68	67.96	15.00
90	VAL	C	0.11	50.36	66.90	15.00
90	VAL	O	-0.09	50.40	65.68	15.00
91	GLY	N	1.05	49.58	67.43	15.00

TABLE X

91 GLY CA	1.85	48.75	66.55	15.00
91 GLY C	3.14	49.42	66.11	15.00
91 GLY O	3.81	48.92	65.19	15.00
92 GLN N	3.51	50.52	66.75	15.00
92 GLN CA	4.75	51.17	66.39	15.00
92 GLN CB	4.53	52.11	65.23	15.00
92 GLN CG	3.31	52.97	65.48	15.00
92 GLN CD	3.44	54.31	64.81	15.00
92 GLN OE1	2.68	54.64	63.92	15.00
92 GLN NE2	4.41	55.10	65.25	15.00
92 GLN C	5.34	51.97	67.53	15.00
92 GLN O	4.72	52.25	68.53	15.00
93 GLU N	6.57	52.40	67.30	15.00
93 GLU CA	7.33	53.20	68.25	15.00
93 GLU CB	8.81	53.08	67.91	15.00
93 GLU CG	9.33	51.65	68.15	15.00
93 GLU CD	10.59	51.29	67.38	15.00
93 GLU OE1	10.87	51.94	66.34	15.00
93 GLU OE2	11.31	50.35	67.80	15.00
93 GLU C	6.85	54.66	68.26	15.00
93 GLU O	6.48	55.24	67.24	15.00
94 GLU N	6.79	55.20	69.46	15.00
94 GLU CA	6.36	56.56	69.67	15.00
94 GLU CB	4.83	56.70	69.62	15.00
94 GLU CG	4.07	55.48	70.04	15.00
94 GLU CD	2.76	55.78	70.70	15.00
94 GLU OE1	1.99	56.60	70.14	15.00
94 GLU OE2	2.51	55.26	71.81	15.00
94 GLU C	6.86	56.98	71.01	15.00
94 GLU O	7.15	56.12	71.84	15.00
95 SER N	6.98	58.29	71.23	15.00
95 SER CA	7.47	58.78	72.52	15.00
95 SER CB	7.26	60.29	72.63	15.00
95 SER OG	6.14	60.73	71.85	15.00
95 SER C	6.78	58.06	73.70	15.00
95 SER O	5.61	57.59	73.59	15.00
96 CYS N	7.52	57.90	74.80	15.00
96 CYS CA	6.93	57.30	75.96	15.00
96 CYS C	5.80	58.23	76.33	15.00
96 CYS O	6.00	59.44	76.37	15.00
96 CYS CB	7.95	57.27	77.09	15.00
96 CYS SG	7.32	56.63	78.67	15.00
97 MET N	4.58	57.73	76.42	15.00

TABLE X

97 MET CA	3.46	58.59	76.84	15.00
97 MET CB	2.40	58.64	75.75	15.00
97 MET CG	2.95	58.79	74.35	15.00
97 MET SD	1.74	59.21	73.09	15.00
97 MET CE	0.27	58.48	73.83	15.00
97 MET C	2.79	58.10	78.14	15.00
97 MET O	1.57	58.06	78.24	15.00
98 TYR N	3.59	57.79	79.15	15.00
98 TYR CA	3.09	57.31	80.45	15.00
98 TYR CB	4.25	56.91	81.37	15.00
98 TYR CG	3.71	56.31	82.64	15.00
98 TYR CD1	2.99	55.13	82.59	15.00
98 TYR CE1	2.42	54.60	83.75	15.00
98 TYR CD2	3.86	56.96	83.88	15.00
98 TYR CE2	3.30	56.45	85.03	15.00
98 TYR CZ	2.59	55.27	84.95	15.00
98 TYR OH	1.99	54.70	86.05	15.00
98 TYR C	2.17	58.29	81.19	15.00
98 TYR O	2.56	59.42	81.48	15.00
99 ASN N	0.97	57.85	81.49	15.00
99 ASN CA	-0.01	58.66	82.21	15.00
99 ASN CB	-1.39	58.64	81.52	15.00
99 ASN CG	-2.41	59.49	82.25	15.00
99 ASN OD1	-2.15	59.98	83.35	15.00
99 ASN ND2	-3.60	59.65	81.65	15.00
99 ASN C	-0.17	58.09	83.63	15.00
99 ASN O	-0.87	57.05	83.81	15.00
100 PRO N	0.31	58.84	84.66	15.00
100 PRO CD	0.81	60.23	84.63	15.00
100 PRO CA	0.20	58.38	86.04	15.00
100 PRO CB	0.80	59.53	86.83	15.00
100 PRO CG	1.64	60.28	85.79	15.00
100 PRO C	-1.25	58.14	86.50	15.00
100 PRO O	-1.49	57.37	87.41	15.00
101 THR N	-2.22	58.73	85.82	15.00
101 THR CA	-3.61	58.53	86.23	15.00
101 THR CB	-4.58	59.63	85.74	15.00
101 THR OG1	-5.12	59.28	84.45	15.00
101 THR CG2	-3.91	60.96	85.67	15.00
101 THR C	-4.09	57.21	85.69	15.00
101 THR O	-5.05	56.64	86.24	15.00
102 GLY N	-3.50	56.77	84.58	15.00
102 GLY CA	-3.90	55.51	83.98	15.00

TABLE X

102	GLY	C	-3.31	54.30	84.66	15.00
102	GLY	O	-3.63	53.16	84.25	15.00
103	LYS	N	-2.50	54.52	85.70	15.00
103	LYS	CA	-1.87	53.41	86.40	15.00
103	LYS	CB	-1.06	53.93	87.58	15.00
103	LYS	CG	-0.26	52.86	88.29	15.00
103	LYS	CD	-0.09	53.20	89.77	15.00
103	LYS	CE	-1.41	52.95	90.56	15.00
103	LYS	NZ	-1.62	51.48	90.82	15.00
103	LYS	C	-2.90	52.38	86.85	15.00
103	LYS	O	-3.84	52.70	87.56	15.00
104	ALA	N	-2.70	51.13	86.45	15.00
104	ALA	CA	-3.60	50.03	86.82	15.00
104	ALA	CB	-4.23	49.45	85.59	15.00
104	ALA	C	-2.81	48.95	87.53	15.00
104	ALA	O	-3.37	48.03	88.10	15.00
105	ALA	N	-1.49	49.07	87.52	15.00
105	ALA	CA	-0.72	48.05	88.20	15.00
105	ALA	CB	-0.65	46.80	87.34	15.00
105	ALA	C	0.66	48.46	88.70	15.00
105	ALA	O	1.21	49.47	88.26	15.00
106	LYS	N	1.18	47.64	89.63	15.00
106	LYS	CA	2.49	47.81	90.27	15.00
106	LYS	CB	2.33	48.37	91.70	15.00
106	LYS	CG	1.94	49.82	91.78	15.00
106	LYS	CD	2.39	50.49	93.08	15.00
106	LYS	CE	3.90	50.73	93.15	15.00
106	LYS	NZ	4.68	49.45	93.03	15.00
106	LYS	C	3.31	46.52	90.33	15.00
106	LYS	O	2.78	45.42	90.25	15.00
107	CYS	N	4.58	46.66	90.67	15.00
107	CYS	CA	5.44	45.50	90.73	15.00
107	CYS	CB	5.96	45.28	89.31	15.00
107	CYS	SG	7.11	43.91	89.12	15.00
107	CYS	C	6.58	45.74	91.71	15.00
107	CYS	O	7.13	46.84	91.75	15.00
108	ARG	N	6.93	44.73	92.50	15.00
108	ARG	CA	8.03	44.94	93.42	15.00
108	ARG	CB	7.57	44.79	94.87	15.00
108	ARG	CG	7.03	43.41	95.26	15.00
108	ARG	CD	6.66	43.37	96.77	15.00
108	ARG	NE	6.16	42.05	97.15	15.00
108	ARG	CZ	6.83	40.90	96.99	15.00

TABLE X

108 ARG NH1	8.05	40.88	96.47	15.00
108 ARG NH2	6.25	39.76	97.31	15.00
108 ARG C	9.24	44.06	93.14	15.00
108 ARG O	9.94	43.63	94.07	15.00
109 GLY N	9.47	43.78	91.85	15.00
109 GLY CA	10.58	42.92	91.49	15.00
109 GLY C	10.15	41.85	90.50	15.00
109 GLY O	9.05	41.91	89.95	15.00
110 TYR N	10.97	40.81	90.37	15.00
110 TYR CA	10.68	39.71	89.47	15.00
110 TYR CB	10.79	40.15	88.01	15.00
110 TYR CG	12.20	40.50	87.61	15.00
110 TYR CD1	12.66	41.85	87.79	15.00
110 TYR CE1	13.95	42.21	87.41	15.00
110 TYR CD2	13.08	39.49	87.02	15.00
110 TYR CE2	14.35	39.80	86.64	15.00
110 TYR CZ	14.80	41.19	86.83	15.00
110 TYR OH	16.07	41.57	86.47	15.00
110 TYR C	11.67	38.57	89.72	15.00
110 TYR O	12.72	38.78	90.34	15.00
111 ARG N	11.36	37.37	89.26	15.00
111 ARG CA	12.26	36.23	89.43	15.00
111 ARG CB	11.86	35.41	90.67	15.00
111 ARG CG	11.78	36.26	91.94	15.00
111 ARG CD	12.04	35.36	93.15	15.00
111 ARG NE	13.43	34.92	93.18	15.00
111 ARG CZ	13.89	33.89	93.89	15.00
111 ARG NH1	15.19	33.60	93.83	15.00
111 ARG NH2	13.04	33.14	94.59	15.00
111 ARG C	12.24	35.31	88.24	15.00
111 ARG O	11.17	35.05	87.66	15.00
112 GLU N	13.43	34.83	87.90	15.00
112 GLU CA	13.63	33.90	86.82	15.00
112 GLU CB	15.09	33.97	86.40	15.00
112 GLU CG	15.46	35.25	85.64	15.00
112 GLU CD	15.38	35.07	84.12	15.00
112 GLU OE1	14.25	35.12	83.56	15.00
112 GLU OE2	16.47	34.88	83.50	15.00
112 GLU C	13.36	32.48	87.30	15.00
112 GLU O	13.00	32.27	88.44	15.00
113 ILE N	13.55	31.53	86.41	15.00
113 ILE CA	13.36	30.12	86.72	15.00
113 ILE CB	12.20	29.54	85.92	15.00

TABLE X

113	ILE	CG2	12.22	28.02	85.90	15.00
113	ILE	CG1	10.91	30.06	86.51	15.00
113	ILE	CD1	9.69	29.82	85.68	15.00
113	ILE	C	14.68	29.49	86.33	15.00
113	ILE	O	15.33	29.97	85.44	15.00
114	PRO	N	15.20	28.55	87.13	15.00
114	PRO	CD	14.60	28.07	88.38	15.00
114	PRO	CA	16.49	27.87	86.88	15.00
114	PRO	CB	16.38	26.62	87.77	15.00
114	PRO	CG	15.73	27.17	88.97	15.00
114	PRO	C	16.69	27.54	85.40	15.00
114	PRO	O	15.93	26.78	84.83	15.00
115	GLU	N	17.71	28.13	84.80	15.00
115	GLU	CA	18.03	28.00	83.38	15.00
115	GLU	CB	19.41	28.59	83.11	15.00
115	GLU	CG	19.58	29.05	81.64	15.00
115	GLU	CD	20.85	29.87	81.42	15.00
115	GLU	OE1	20.80	31.11	81.48	15.00
115	GLU	OE2	21.91	29.28	81.19	15.00
115	GLU	C	17.96	26.62	82.77	15.00
115	GLU	O	18.99	25.96	82.65	15.00
116	GLY	N	16.78	26.24	82.28	15.00
116	GLY	CA	16.64	24.93	81.66	15.00
116	GLY	C	15.95	23.89	82.52	15.00
116	GLY	O	15.82	22.73	82.13	15.00
117	ASN	N	15.49	24.30	83.70	15.00
117	ASN	CA	14.84	23.38	84.61	15.00
117	ASN	CB	15.29	23.66	86.03	15.00
117	ASN	CG	14.55	22.85	87.06	15.00
117	ASN	OD1	13.47	22.36	86.81	15.00
117	ASN	ND2	15.14	22.73	88.25	15.00
117	ASN	C	13.34	23.50	84.47	15.00
117	ASN	O	12.71	24.37	85.05	15.00
118	GLU	N	12.78	22.55	83.74	15.00
118	GLU	CA	11.35	22.52	83.45	15.00
118	GLU	CB	11.10	21.52	82.33	15.00
118	GLU	CG	10.04	21.91	81.37	15.00
118	GLU	CD	9.94	20.95	80.16	15.00
118	GLU	OE1	8.82	20.50	79.88	15.00
118	GLU	OE2	10.96	20.58	79.52	15.00
118	GLU	C	10.45	22.18	84.64	15.00
118	GLU	O	9.30	22.61	84.67	15.00
119	LYS	N	10.97	21.46	85.63	15.00

TABLE X

119	LYS	CA	10.15	21.13	86.77	15.00
119	LYS	CB	10.74	19.95	87.52	15.00
119	LYS	CG	9.69	19.04	88.07	15.00
119	LYS	CD	8.84	18.47	86.94	15.00
119	LYS	CE	7.78	17.54	87.45	15.00
119	LYS	NZ	7.03	17.08	86.28	15.00
119	LYS	C	10.02	22.33	87.69	15.00
119	LYS	O	9.02	22.45	88.42	15.00
120	ALA	N	11.01	23.22	87.66	15.00
120	ALA	CA	10.99	24.43	88.48	15.00
120	ALA	CB	12.36	25.05	88.46	15.00
120	ALA	C	9.95	25.39	87.87	15.00
120	ALA	O	9.39	26.27	88.57	15.00
121	LEU	N	9.79	25.27	86.55	15.00
121	LEU	CA	8.83	26.05	85.78	15.00
121	LEU	CB	9.06	25.87	84.28	15.00
121	LEU	CG	8.06	26.54	83.31	15.00
121	LEU	CD1	8.05	28.02	83.54	15.00
121	LEU	CD2	8.42	26.24	81.90	15.00
121	LEU	C	7.43	25.59	86.13	15.00
121	LEU	O	6.59	26.43	86.46	15.00
122	LYS	N	7.17	24.28	86.10	15.00
122	LYS	CA	5.83	23.74	86.40	15.00
122	LYS	CB	5.81	22.20	86.25	15.00
122	LYS	CG	4.49	21.54	86.59	15.00
122	LYS	CD	4.61	20.10	86.92	15.00
122	LYS	CE	5.26	19.90	88.29	15.00
122	LYS	NZ	5.14	18.48	88.78	15.00
122	LYS	C	5.34	24.13	87.78	15.00
122	LYS	O	4.13	24.20	87.99	15.00
123	ARG	N	6.27	24.36	88.71	15.00
123	ARG	CA	5.90	24.76	90.06	15.00
123	ARG	CB	6.95	24.36	91.07	15.00
123	ARG	CG	7.05	22.94	91.45	15.00
123	ARG	CD	8.15	22.86	92.43	15.00
123	ARG	NE	9.44	23.25	91.82	15.00
123	ARG	CZ	10.56	23.53	92.50	15.00
123	ARG	NH1	10.58	23.50	93.81	15.00
123	ARG	NH2	11.71	23.76	91.85	15.00
123	ARG	C	5.71	26.25	90.17	15.00
123	ARG	O	5.12	26.72	91.13	15.00
124	ALA	N	6.31	27.00	89.25	15.00
124	ALA	CA	6.16	28.42	89.30	15.00

TABLE X

124 ALA CB	7.22	29.12	88.43	15.00
124 ALA C	4.78	28.73	88.81	15.00
124 ALA O	4.06	29.46	89.47	15.00
125 VAL N	4.37	28.09	87.72	15.00
125 VAL CA	3.06	28.41	87.21	15.00
125 VAL CB	2.82	27.94	85.72	15.00
125 VAL CG1	4.09	27.54	85.00	15.00
125 VAL CG2	1.70	26.88	85.60	15.00
125 VAL C	2.03	27.82	88.15	15.00
125 VAL O	0.89	28.28	88.17	15.00
126 ALA N	2.42	26.86	88.98	15.00
126 ALA CA	1.47	26.25	89.89	15.00
126 ALA CB	1.94	24.91	90.29	15.00
126 ALA C	1.32	27.11	91.12	15.00
126 ALA O	0.22	27.27	91.63	15.00
127 ARG N	2.42	27.71	91.55	15.00
127 ARG CA	2.42	28.50	92.77	15.00
127 ARG CB	3.67	28.22	93.60	15.00
127 ARG CG	3.74	26.79	94.07	15.00
127 ARG CD	5.07	26.45	94.67	15.00
127 ARG NE	5.02	25.01	94.96	15.00
127 ARG CZ	6.03	24.24	95.34	15.00
127 ARG NH1	5.84	22.94	95.55	15.00
127 ARG NH2	7.24	24.73	95.54	15.00
127 ARG C	2.30	29.98	92.61	15.00
127 ARG O	2.15	30.68	93.60	15.00
128 VAL N	2.46	30.47	91.38	15.00
128 VAL CA	2.37	31.91	91.11	15.00
128 VAL CB	3.70	32.49	90.59	15.00
128 VAL CG1	3.62	33.98	90.47	15.00
128 VAL CG2	4.87	32.10	91.53	15.00
128 VAL C	1.29	32.25	90.10	15.00
128 VAL O	0.47	33.10	90.36	15.00
129 GLY N	1.30	31.60	88.94	15.00
129 GLY CA	0.31	31.85	87.91	15.00
129 GLY C	1.10	32.00	86.61	15.00
129 GLY O	2.27	31.60	86.57	15.00
130 PRO N	0.52	32.56	85.53	15.00
130 PRO CD	-0.89	32.96	85.30	15.00
130 PRO CA	1.27	32.70	84.30	15.00
130 PRO CB	0.38	33.61	83.50	15.00
130 PRO CG	-0.98	33.09	83.81	15.00
130 PRO C	2.68	33.24	84.44	15.00

TABLE X

130	PRO O	2.93	34.17	85.20	15.00
131	VAL N	3.59	32.56	83.75	15.00
131	VAL CA	5.01	32.88	83.76	15.00
131	VAL CB	5.79	31.64	84.27	15.00
131	VAL CG1	7.25	31.88	84.32	15.00
131	VAL CG2	5.29	31.20	85.62	15.00
131	VAL C	5.46	33.28	82.34	15.00
131	VAL O	4.93	32.82	81.36	15.00
132	SER N	6.29	34.30	82.27	15.00
132	SER CA	6.77	34.75	80.98	15.00
132	SER CB	7.15	36.24	81.04	15.00
132	SER OG	5.98	36.98	81.39	15.00
132	SER C	7.92	33.89	80.48	15.00
132	SER O	9.01	33.83	81.08	15.00
133	VAL N	7.65	33.20	79.38	15.00
133	VAL CA	8.65	32.34	78.76	15.00
133	VAL CB	8.09	30.90	78.61	15.00
133	VAL CG1	7.58	30.35	79.92	15.00
133	VAL CG2	6.97	30.91	77.61	15.00
133	VAL C	9.05	32.84	77.37	15.00
133	VAL O	8.48	33.81	76.85	15.00
134	ALA N	10.08	32.21	76.81	15.00
134	ALA CA	10.60	32.51	75.49	15.00
134	ALA CB	11.89	33.29	75.59	15.00
134	ALA C	10.85	31.16	74.84	15.00
134	ALA O	11.46	30.30	75.47	15.00
135	ILE N	10.35	30.97	73.62	15.00
135	ILE CA	10.52	29.73	72.86	15.00
135	ILE CB	9.18	28.95	72.80	15.00
135	ILE CG2	8.71	28.60	74.21	15.00
135	ILE CG1	8.13	29.80	72.09	15.00
135	ILE CD1	6.78	29.14	72.00	15.00
135	ILE C	11.04	30.04	71.44	15.00
135	ILE O	11.30	31.20	71.08	15.00
136	ASP N	11.28	28.98	70.67	15.00
136	ASP CA	11.71	29.13	69.30	15.00
136	ASP CB	12.68	28.01	68.94	15.00
136	ASP CG	13.21	28.11	67.50	15.00
136	ASP OD1	13.77	27.12	67.00	15.00
136	ASP OD2	13.08	29.18	66.88	15.00
136	ASP C	10.45	28.94	68.51	15.00
136	ASP O	9.90	27.82	68.48	15.00
137	ALA N	9.98	30.01	67.87	15.00

TABLE X

137	ALA	CA	8.78	29.93	67.06	15.00
137	ALA	CB	7.74	30.91	67.56	15.00
137	ALA	C	9.09	30.18	65.58	15.00
137	ALA	O	8.27	30.79	64.88	15.00
138	SER	N	10.22	29.67	65.10	15.00
138	SER	CA	10.66	29.83	63.72	15.00
138	SER	CB	12.18	29.81	63.63	15.00
138	SER	OG	12.67	28.54	64.01	15.00
138	SER	C	10.15	28.77	62.77	15.00
138	SER	O	9.81	29.07	61.62	15.00
139	LEU	N	10.12	27.53	63.26	15.00
139	LEU	CA	9.66	26.42	62.45	15.00
139	LEU	CB	9.74	25.13	63.29	15.00
139	LEU	CG	11.05	24.33	63.34	15.00
139	LEU	CD1	12.24	25.24	63.67	15.00
139	LEU	CD2	10.92	23.21	64.38	15.00
139	LEU	C	8.24	26.59	61.88	15.00
139	LEU	O	7.32	26.95	62.60	15.00
140	THR	N	8.08	26.30	60.58	15.00
140	THR	CA	6.80	26.39	59.88	15.00
140	THR	CB	6.88	25.76	58.50	15.00
140	THR	OG1	8.18	25.97	57.94	15.00
140	THR	CG2	5.86	26.37	57.60	15.00
140	THR	C	5.76	25.62	60.67	15.00
140	THR	O	4.67	26.12	60.88	15.00
141	SER	N	6.13	24.45	61.17	15.00
141	SER	CA	5.20	23.63	61.94	15.00
141	SER	CB	5.79	22.28	62.28	15.00
141	SER	OG	7.00	22.40	62.97	15.00
141	SER	C	4.65	24.28	63.18	15.00
141	SER	O	3.60	23.89	63.66	15.00
142	PHE	N	5.35	25.26	63.72	15.00
142	PHE	CA	4.82	25.94	64.90	15.00
142	PHE	CB	5.94	26.71	65.64	15.00
142	PHE	CG	5.46	27.49	66.86	15.00
142	PHE	CD1	5.60	26.99	68.12	15.00
142	PHE	CD2	4.89	28.74	66.71	15.00
142	PHE	CE1	5.15	27.76	69.25	15.00
142	PHE	CE2	4.46	29.49	67.82	15.00
142	PHE	CZ	4.59	29.00	69.07	15.00
142	PHE	C	3.74	26.88	64.42	15.00
142	PHE	O	2.63	26.88	64.93	15.00
143	GLN	N	4.08	27.58	63.36	15.00

TABLE X

143	GLN	CA	3.24	28.59	62.73	15.00
143	GLN	CB	4.04	29.36	61.69	15.00
143	GLN	CG	5.38	29.87	62.23	15.00
143	GLN	CD	6.19	30.64	61.16	15.00
143	GLN	OE1	5.83	31.75	60.75	15.00
143	GLN	NE2	7.25	30.01	60.64	15.00
143	GLN	C	1.95	28.10	62.12	15.00
143	GLN	O	0.99	28.86	62.08	15.00
144	PHE	N	1.91	26.90	61.55	15.00
144	PHE	CA	0.61	26.44	61.01	15.00
144	PHE	CB	0.73	25.77	59.63	15.00
144	PHE	CG	1.72	24.62	59.58	15.00
144	PHE	CD1	2.76	24.61	58.69	15.00
144	PHE	CD2	1.58	23.50	60.36	15.00
144	PHE	CE1	3.60	23.51	58.60	15.00
144	PHE	CE2	2.47	22.41	60.22	15.00
144	PHE	CZ	3.44	22.44	59.35	15.00
144	PHE	C	-0.14	25.50	61.98	15.00
144	PHE	O	-1.10	24.82	61.59	15.00
145	TYR	N	0.31	25.47	63.24	15.00
145	TYR	CA	-0.31	24.65	64.26	15.00
145	TYR	CB	0.32	24.91	65.65	15.00
145	TYR	CG	-0.47	24.34	66.81	15.00
145	TYR	CD1	-0.26	23.01	67.22	15.00
145	TYR	CE1	-0.98	22.48	68.28	15.00
145	TYR	CD2	-1.42	25.12	67.48	15.00
145	TYR	CE2	-2.15	24.61	68.54	15.00
145	TYR	CZ	-1.93	23.28	68.94	15.00
145	TYR	OH	-2.67	22.83	70.02	15.00
145	TYR	C	-1.80	24.98	64.30	15.00
145	TYR	O	-2.24	26.10	64.03	15.00
146	SER	N	-2.60	24.00	64.69	15.00
146	SER	CA	-4.06	24.19	64.77	15.00
146	SER	CB	-4.67	23.67	63.48	15.00
146	SER	OG	-4.29	22.33	63.27	15.00
146	SER	C	-4.67	23.42	65.95	15.00
146	SER	O	-5.59	23.89	66.62	15.00
147	LYS	N	-4.20	22.20	66.13	15.00
147	LYS	CA	-4.67	21.36	67.20	15.00
147	LYS	CB	-5.96	20.64	66.83	15.00
147	LYS	CG	-5.81	19.47	65.90	15.00
147	LYS	CD	-7.06	18.58	65.92	15.00
147	LYS	CE	-6.91	17.41	64.96	15.00

TABLE X

147	LYS	NZ	-8.13	16.56	64.99	15.00
147	LYS	C	-3.60	20.36	67.62	15.00
147	LYS	O	-2.62	20.16	66.90	15.00
148	GLY	N	-3.82	19.73	68.78	15.00
148	GLY	CA	-2.88	18.75	69.30	15.00
148	GLY	C	-1.76	19.26	70.20	15.00
148	GLY	O	-1.75	20.39	70.59	15.00
149	VAL	N	-0.79	18.40	70.52	15.00
149	VAL	CA	0.33	18.81	71.35	15.00
149	VAL	CB	0.58	17.89	72.57	15.00
149	VAL	CG1	1.74	18.42	73.41	15.00
149	VAL	CG2	-0.68	17.75	73.42	15.00
149	VAL	C	1.59	18.86	70.48	15.00
149	VAL	O	2.06	17.84	69.96	15.00
150	TYR	N	2.13	20.07	70.35	15.00
150	TYR	CA	3.32	20.33	69.53	15.00
150	TYR	CB	3.50	21.83	69.29	15.00
150	TYR	CG	4.59	22.21	68.31	15.00
150	TYR	CD1	4.47	22.01	66.95	15.00
150	TYR	CE1	5.48	22.37	66.04	15.00
150	TYR	CD2	5.74	22.78	68.72	15.00
150	TYR	CE2	6.75	23.13	67.81	15.00
150	TYR	CZ	6.61	22.93	66.48	15.00
150	TYR	OH	7.57	23.30	65.60	15.00
150	TYR	C	4.60	19.72	70.12	15.00
150	TYR	O	4.76	19.60	71.37	15.00
151	TYR	N	5.44	19.24	69.21	15.00
151	TYR	CA	6.74	18.68	69.55	15.00
151	TYR	CB	6.62	17.30	70.22	15.00
151	TYR	CG	7.96	16.61	70.42	15.00
151	TYR	CD1	9.15	17.34	70.60	15.00
151	TYR	CE1	10.41	16.67	70.84	15.00
151	TYR	CD2	8.02	15.21	70.47	15.00
151	TYR	CE2	9.24	14.52	70.71	15.00
151	TYR	CZ	10.43	15.27	70.89	15.00
151	TYR	OH	11.60	14.61	71.14	15.00
151	TYR	C	7.38	18.53	68.19	15.00
151	TYR	O	6.82	17.86	67.31	15.00
152	ASP	N	8.47	19.26	67.98	15.00
152	ASP	CA	9.18	19.22	66.71	15.00
152	ASP	CB	8.83	20.40	65.81	15.00
152	ASP	CG	9.30	20.18	64.37	15.00
152	ASP	OD1	10.54	20.06	64.18	15.00

TABLE X

152 ASP OD2	8.42	20.06	63.48	15.00
152 ASP C	10.69	19.18	66.97	15.00
152 ASP O	11.34	20.21	67.14	15.00
153 GLU N	11.24	17.97	66.94	15.00
153 GLU CA	12.64	17.77	67.18	15.00
153 GLU CB	13.00	16.30	66.88	15.00
153 GLU CG	12.45	15.71	65.61	15.00
153 GLU CD	11.10	15.02	65.83	15.00
153 GLU OE1	11.10	13.96	66.53	15.00
153 GLU OE2	10.06	15.52	65.30	15.00
153 GLU C	13.60	18.73	66.48	15.00
153 GLU O	14.75	18.90	66.91	15.00
154 SER N	13.17	19.30	65.35	15.00
154 SER CA	14.02	20.24	64.60	15.00
154 SER CB	13.49	20.49	63.17	15.00
154 SER OG	13.06	19.29	62.54	15.00
154 SER C	14.13	21.57	65.34	15.00
154 SER O	14.95	22.40	65.00	15.00
155 CYS N	13.37	21.72	66.43	15.00
155 CYS CA	13.33	22.98	67.21	15.00
155 CYS C	14.64	23.18	67.97	15.00
155 CYS O	15.25	22.21	68.44	15.00
155 CYS CB	12.15	22.99	68.17	15.00
155 CYS SG	11.63	24.66	68.64	15.00
156 ASN N	15.04	24.44	68.16	15.00
156 ASN CA	16.31	24.74	68.81	15.00
156 ASN CB	17.20	25.46	67.80	15.00
156 ASN CG	18.46	26.05	68.41	15.00
156 ASN OD1	18.80	25.83	69.59	15.00
156 ASN ND2	19.18	26.80	67.59	15.00
156 ASN C	16.22	25.55	70.11	15.00
156 ASN O	16.12	26.80	70.09	15.00
157 SER N	16.27	24.83	71.22	15.00
157 SER CA	16.22	25.44	72.55	15.00
157 SER CB	16.51	24.37	73.60	15.00
157 SER OG	15.49	23.40	73.56	15.00
157 SER C	17.22	26.59	72.72	15.00
157 SER O	16.99	27.51	73.49	15.00
158 ASP N	18.35	26.52	72.02	15.00
158 ASP CA	19.40	27.52	72.06	15.00
158 ASP CB	20.71	26.91	71.57	15.00
158 ASP CG	20.91	25.47	72.03	15.00
158 ASP OD1	21.16	24.60	71.16	15.00

TABLE X

158 ASP OD2	20.81	25.18	73.26	15.00
158 ASP C	19.05	28.77	71.26	15.00
158 ASP O	19.69	29.81	71.37	15.00
159 ASN N	18.04	28.67	70.40	15.00
159 ASN CA	17.64	29.82	69.62	15.00
159 ASN CB	17.77	29.53	68.12	15.00
159 ASN CG	17.54	30.78	67.23	15.00
159 ASN OD1	17.33	30.67	66.00	15.00
159 ASN ND2	17.63	31.96	67.83	15.00
159 ASN C	16.22	30.27	69.99	15.00
159 ASN O	15.23	29.87	69.36	15.00
160 LEU N	16.12	31.10	71.03	15.00
160 LEU CA	14.84	31.64	71.49	15.00
160 LEU CB	14.88	31.87	73.00	15.00
160 LEU CG	15.40	30.70	73.88	15.00
160 LEU CD1	15.23	31.09	75.33	15.00
160 LEU CD2	14.68	29.38	73.59	15.00
160 LEU C	14.66	32.96	70.75	15.00
160 LEU O	15.56	33.76	70.75	15.00
161 ASN N	13.52	33.17	70.11	15.00
161 ASN CA	13.28	34.40	69.36	15.00
161 ASN CB	13.53	34.18	67.85	15.00
161 ASN CG	12.91	32.90	67.32	15.00
161 ASN OD1	11.68	32.70	67.33	15.00
161 ASN ND2	13.78	32.01	66.83	15.00
161 ASN C	11.86	34.98	69.54	15.00
161 ASN O	11.57	36.09	69.09	15.00
162 HIS N	10.99	34.28	70.26	15.00
162 HIS CA	9.66	34.79	70.41	15.00
162 HIS CB	8.74	34.04	69.45	15.00
162 HIS CG	7.37	34.62	69.35	15.00
162 HIS CD2	6.94	35.88	69.10	15.00
162 HIS ND1	6.24	33.84	69.45	15.00
162 HIS CE1	5.17	34.59	69.25	15.00
162 HIS NE2	5.57	35.83	69.03	15.00
162 HIS C	9.28	34.53	71.85	15.00
162 HIS O	9.61	33.48	72.39	15.00
163 ALA N	8.70	35.56	72.47	15.00
163 ALA CA	8.26	35.51	73.85	15.00
163 ALA CB	8.50	36.80	74.53	15.00
163 ALA C	6.78	35.24	73.87	15.00
163 ALA O	6.02	35.80	73.09	15.00
164 VAL N	6.39	34.38	74.78	15.00

TABLE X

164 VAL CA	5.01	34.03	74.97	15.00
164 VAL CB	4.69	32.69	74.29	15.00
164 VAL CG1	4.67	32.84	72.75	15.00
164 VAL CG2	5.73	31.64	74.69	15.00
164 VAL C	4.72	33.94	76.48	15.00
164 VAL O	5.55	34.42	77.30	15.00
165 LEU N	3.60	33.31	76.85	15.00
165 LEU CA	3.27	33.21	78.26	15.00
165 LEU CB	2.31	34.36	78.60	15.00
165 LEU CG	1.52	34.51	79.93	15.00
165 LEU CD1	2.25	35.21	81.00	15.00
165 LEU CD2	0.26	35.25	79.65	15.00
165 LEU C	2.65	31.88	78.63	15.00
165 LEU O	1.68	31.50	77.98	15.00
166 ALA N	3.25	31.15	79.57	15.00
166 ALA CA	2.73	29.85	80.03	15.00
166 ALA CB	3.79	29.05	80.72	15.00
166 ALA C	1.57	30.12	80.98	15.00
166 ALA O	1.76	30.63	82.05	15.00
167 VAL N	0.38	29.73	80.56	15.00
167 VAL CA	-0.88	29.95	81.26	15.00
167 VAL CB	-1.94	30.48	80.19	15.00
167 VAL CG1	-3.36	30.02	80.45	15.00
167 VAL CG2	-1.88	32.03	80.10	15.00
167 VAL C	-1.36	28.70	82.03	15.00
167 VAL O	-2.35	28.75	82.70	15.00
168 GLY N	-0.67	27.57	81.88	15.00
168 GLY CA	-1.07	26.35	82.56	15.00
168 GLY C	-0.36	25.13	82.00	15.00
168 GLY O	0.52	25.29	81.17	15.00
169 TYR N	-0.68	23.94	82.49	15.00
169 TYR CA	-0.03	22.73	81.98	15.00
169 TYR CB	1.33	22.45	82.69	15.00
169 TYR CG	1.24	22.33	84.21	15.00
169 TYR CD1	0.66	21.21	84.82	15.00
169 TYR CE1	0.51	21.16	86.19	15.00
169 TYR CD2	1.67	23.36	85.02	15.00
169 TYR CE2	1.53	23.30	86.36	15.00
169 TYR CZ	0.94	22.20	86.95	15.00
169 TYR OH	0.76	22.18	88.32	15.00
169 TYR C	-0.97	21.62	82.29	15.00
169 TYR O	-1.89	21.79	83.08	15.00
170 GLY N	-0.71	20.47	81.70	15.00

TABLE X

170 GLY CA	-1.54	19.31	81.93	15.00
170 GLY C	-1.19	18.20	80.97	15.00
170 GLY O	-0.05	18.05	80.56	15.00
171 ILE N	-2.19	17.42	80.63	15.00
171 ILE CA	-1.99	16.31	79.71	15.00
171 ILE CB	-1.71	14.98	80.49	15.00
171 ILE CG2	-2.84	14.65	81.48	15.00
171 ILE CG1	-1.47	13.80	79.57	15.00
171 ILE CD1	-1.37	12.49	80.30	15.00
171 ILE C	-3.23	16.19	78.81	15.00
171 ILE O	-4.29	16.77	79.10	15.00
172 GLN N	-3.09	15.50	77.69	15.00
172 GLN CA	-4.21	15.35	76.77	15.00
172 GLN CB	-3.96	16.16	75.48	15.00
172 GLN CG	-5.15	16.20	74.49	15.00
172 GLN CD	-5.05	17.33	73.50	15.00
172 GLN OE1	-4.76	18.47	73.87	15.00
172 GLN NE2	-5.27	17.03	72.22	15.00
172 GLN C	-4.51	13.86	76.49	15.00
172 GLN O	-5.23	13.22	77.27	15.00
173 LYS N	-4.00	13.30	75.41	15.00
173 LYS CA	-4.27	11.89	75.22	15.00
173 LYS CB	-4.76	11.64	73.81	15.00
173 LYS CG	-6.07	12.36	73.52	15.00
173 LYS CD	-6.45	12.30	72.03	15.00
173 LYS CE	-5.44	13.01	71.15	15.00
173 LYS NZ	-5.85	12.96	69.72	15.00
173 LYS C	-2.97	11.18	75.51	15.00
173 LYS O	-2.29	10.72	74.59	15.00
174 GLY N	-2.59	11.22	76.78	15.00
174 GLY CA	-1.36	10.60	77.21	15.00
174 GLY C	-0.18	11.54	77.14	15.00
174 GLY O	0.88	11.27	77.72	15.00
175 ASN N	-0.34	12.66	76.42	15.00
175 ASN CA	0.75	13.62	76.27	15.00
175 ASN CB	0.84	14.07	74.82	15.00
175 ASN CG	1.30	12.97	73.90	15.00
175 ASN OD1	2.46	12.52	73.96	15.00
175 ASN ND2	0.38	12.50	73.05	15.00
175 ASN C	0.75	14.84	77.17	15.00
175 ASN O	-0.24	15.61	77.23	15.00
176 LYS N	1.91	15.07	77.78	15.00
176 LYS CA	2.12	16.20	78.66	15.00

TABLE X

176 LYS CB	3.36	15.99	79.53	15.00
176 LYS CG	3.19	14.86	80.52	15.00
176 LYS CD	4.24	14.85	81.66	15.00
176 LYS CE	4.17	13.51	82.41	15.00
176 LYS NZ	2.95	13.37	83.28	15.00
176 LYS C	2.25	17.46	77.85	15.00
176 LYS O	2.71	17.42	76.71	15.00
177 HIS N	1.74	18.56	78.38	15.00
177 HIS CA	1.85	19.81	77.66	15.00
177 HIS CB	0.73	19.92	76.63	15.00
177 HIS CG	-0.62	20.17	77.21	15.00
177 HIS CD2	-1.20	21.32	77.65	15.00
177 HIS ND1	-1.56	19.18	77.38	15.00
177 HIS CE1	-2.67	19.70	77.89	15.00
177 HIS NE2	-2.47	21.00	78.06	15.00
177 HIS C	1.83	21.03	78.53	15.00
177 HIS O	1.38	20.97	79.68	15.00
178 TRP N	2.20	22.13	77.89	15.00
178 TRP CA	2.21	23.47	78.45	15.00
178 TRP CB	3.57	24.15	78.26	15.00
178 TRP CG	4.71	23.55	78.98	15.00
178 TRP CD2	4.98	23.62	80.41	15.00
178 TRP CE2	6.14	22.88	80.64	15.00
178 TRP CE3	4.33	24.22	81.52	15.00
178 TRP CD1	5.70	22.82	78.45	15.00
178 TRP NE1	6.56	22.40	79.44	15.00
178 TRP CZ2	6.67	22.72	81.91	15.00
178 TRP CZ3	4.86	24.05	82.77	15.00
178 TRP CH2	6.01	23.31	82.96	15.00
178 TRP C	1.18	24.24	77.64	15.00
178 TRP O	1.14	24.11	76.42	15.00
179 ILE N	0.33	25.01	78.30	15.00
179 ILE CA	-0.64	25.81	77.55	15.00
179 ILE CB	-1.90	26.08	78.34	15.00
179 ILE CG2	-2.77	27.07	77.61	15.00
179 ILE CG1	-2.54	24.73	78.71	15.00
179 ILE CD1	-3.79	24.79	79.53	15.00
179 ILE C	0.03	27.14	77.31	15.00
179 ILE O	0.36	27.82	78.27	15.00
180 ILE N	0.23	27.49	76.05	15.00
180 ILE CA	0.89	28.72	75.68	15.00
180 ILE CB	2.09	28.49	74.78	15.00
180 ILE CG2	2.73	29.81	74.51	15.00

TABLE X

180 ILE CG1	3.09	27.57	75.46	15.00
180 ILE CD1	3.92	28.26	76.47	15.00
180 ILE C	-0.04	29.69	75.03	15.00
180 ILE O	-0.88	29.33	74.22	15.00
181 LYS N	0.06	30.94	75.44	15.00
181 LYS CA	-0.80	31.95	74.91	15.00
181 LYS CB	-1.26	32.84	76.03	15.00
181 LYS CG	-1.94	34.09	75.52	15.00
181 LYS CD	-2.47	34.90	76.67	15.00
181 LYS CE	-2.92	36.22	76.11	15.00
181 LYS NZ	-3.47	37.09	77.17	15.00
181 LYS C	0.15	32.72	74.03	15.00
181 LYS O	1.19	33.15	74.52	15.00
182 ASN N	-0.15	32.81	72.75	15.00
182 ASN CA	0.73	33.49	71.81	15.00
182 ASN CB	0.96	32.61	70.59	15.00
182 ASN CG	1.97	33.17	69.65	15.00
182 ASN OD1	2.31	34.34	69.73	15.00
182 ASN ND2	2.42	32.35	68.71	15.00
182 ASN C	0.01	34.76	71.38	15.00
182 ASN O	-1.21	34.83	71.39	15.00
183 SER N	0.75	35.80	71.01	15.00
183 SER CA	0.09	37.03	70.61	15.00
183 SER CB	0.81	38.23	71.20	15.00
183 SER OG	2.19	38.09	71.04	15.00
183 SER C	-0.09	37.18	69.10	15.00
183 SER O	0.19	38.25	68.56	15.00
184 TRP N	-0.58	36.16	68.41	15.00
184 TRP CA	-0.73	36.29	66.97	15.00
184 TRP CB	0.00	35.18	66.21	15.00
184 TRP CG	1.47	35.38	66.20	15.00
184 TRP CD2	2.44	34.39	65.92	15.00
184 TRP CE2	3.69	35.01	65.97	15.00
184 TRP CE3	2.38	33.02	65.61	15.00
184 TRP CD1	2.13	36.54	66.41	15.00
184 TRP NE1	3.47	36.33	66.27	15.00
184 TRP CZ2	4.88	34.32	65.74	15.00
184 TRP CZ3	3.56	32.33	65.37	15.00
184 TRP CH2	4.79	32.98	65.44	15.00
184 TRP C	-2.17	36.42	66.57	15.00
184 TRP O	-2.53	36.20	65.42	15.00
185 GLY N	-2.97	36.92	67.51	15.00
185 GLY CA	-4.37	37.14	67.23	15.00

TABLE X

185 GLY C	-5.06	35.83	67.50	15.00
185 GLY O	-4.46	34.76	67.64	15.00
186 GLU N	-6.37	35.94	67.57	15.00
186 GLU CA	-7.23	34.80	67.84	15.00
186 GLU CB	-8.63	35.32	68.26	15.00
186 GLU CG	-9.57	34.27	68.68	15.00
186 GLU CD	-10.89	34.86	69.09	15.00
186 GLU OE1	-11.68	35.25	68.20	15.00
186 GLU OE2	-11.14	34.91	70.31	15.00
186 GLU C	-7.36	33.76	66.75	15.00
186 GLU O	-7.74	32.62	67.03	15.00
187 ASN N	-7.00	34.14	65.52	15.00
187 ASN CA	-7.11	33.25	64.36	15.00
187 ASN CB	-7.33	34.07	63.08	15.00
187 ASN CG	-8.45	33.50	62.21	15.00
187 ASN OD1	-8.22	33.17	61.07	15.00
187 ASN ND2	-9.66	33.42	62.75	15.00
187 ASN C	-5.92	32.36	64.14	15.00
187 ASN O	-5.90	31.63	63.13	15.00
188 TRP N	-4.89	32.50	64.96	15.00
188 TRP CA	-3.73	31.66	64.83	15.00
188 TRP CB	-2.53	32.41	65.32	15.00
188 TRP CG	-1.34	31.51	65.25	15.00
188 TRP CD2	-0.66	30.87	66.35	15.00
188 TRP CE2	0.34	30.12	65.83	15.00
188 TRP CE3	-0.81	30.87	67.72	15.00
188 TRP CD1	-0.72	31.11	64.13	15.00
188 TRP NE1	0.30	30.26	64.46	15.00
188 TRP CZ2	1.18	29.39	66.64	15.00
188 TRP CZ3	0.04	30.13	68.52	15.00
188 TRP CH2	0.98	29.43	68.01	15.00
188 TRP C	-3.93	30.46	65.72	15.00
188 TRP O	-4.69	30.59	66.69	15.00
189 GLY N	-3.29	29.33	65.40	15.00
189 GLY CA	-3.42	28.14	66.22	15.00
189 GLY C	-4.80	27.88	66.77	15.00
189 GLY O	-5.82	28.15	66.15	15.00
190 ASN N	-4.87	27.38	67.98	15.00
190 ASN CA	-6.16	27.08	68.58	15.00
190 ASN CB	-6.04	25.89	69.53	15.00
190 ASN CG	-7.37	25.28	69.86	15.00
190 ASN OD1	-8.42	25.95	69.81	15.00
190 ASN ND2	-7.34	24.00	70.23	15.00

TABLE X

190 ASN C	-6.70	28.34	69.26	15.00
190 ASN O	-6.57	28.50	70.46	15.00
191 LYS N	-7.23	29.26	68.47	15.00
191 LYS CA	-7.79	30.49	68.99	15.00
191 LYS CB	-9.10	30.17	69.71	15.00
191 LYS CG	-10.01	29.28	68.87	15.00
191 LYS CD	-10.50	29.93	67.53	15.00
191 LYS CE	-9.41	30.19	66.45	15.00
191 LYS NZ	-8.63	28.95	66.03	15.00
191 LYS C	-6.81	31.27	69.84	15.00
191 LYS O	-7.13	31.73	70.96	15.00
192 GLY N	-5.60	31.43	69.30	15.00
192 GLY CA	-4.58	32.18	70.01	15.00
192 GLY C	-3.63	31.36	70.87	15.00
192 GLY O	-2.54	31.86	71.19	15.00
193 TYR N	-4.03	30.16	71.27	15.00
193 TYR CA	-3.20	29.32	72.12	15.00
193 TYR CB	-4.03	28.72	73.28	15.00
193 TYR CG	-4.53	29.79	74.21	15.00
193 TYR CD1	-5.69	30.50	73.91	15.00
193 TYR CE1	-6.13	31.53	74.73	15.00
193 TYR CD2	-3.81	30.13	75.36	15.00
193 TYR CE2	-4.22	31.14	76.20	15.00
193 TYR CZ	-5.37	31.84	75.89	15.00
193 TYR OH	-5.74	32.89	76.71	15.00
193 TYR C	-2.54	28.21	71.35	15.00
193 TYR O	-2.85	27.94	70.17	15.00
194 ILE N	-1.68	27.50	72.06	15.00
194 ILE CA	-0.99	26.35	71.50	15.00
194 ILE CB	0.26	26.72	70.64	15.00
194 ILE CG2	1.18	27.65	71.44	15.00
194 ILE CG1	1.03	25.47	70.15	15.00
194 ILE CD1	2.16	25.76	69.14	15.00
194 ILE C	-0.54	25.54	72.70	15.00
194 ILE O	-0.28	26.08	73.75	15.00
195 LEU N	-0.56	24.23	72.57	15.00
195 LEU CA	-0.12	23.30	73.59	15.00
195 LEU CB	-1.11	22.15	73.67	15.00
195 LEU CG	-2.34	22.29	74.58	15.00
195 LEU CD1	-2.88	23.70	74.67	15.00
195 LEU CD2	-3.41	21.38	74.05	15.00
195 LEU C	1.21	22.81	73.09	15.00
195 LEU O	1.31	22.26	71.99	15.00

TABLE X

196 MET N	2.25	23.13	73.83	15.00
196 MET CA	3.58	22.69	73.45	15.00
196 MET CB	4.57	23.83	73.65	15.00
196 MET CG	4.29	24.99	72.69	15.00
196 MET SD	5.56	26.26	72.94	15.00
196 MET CE	7.08	25.68	71.98	15.00
196 MET C	3.97	21.45	74.27	15.00
196 MET O	3.31	21.15	75.28	15.00
197 ALA N	4.97	20.70	73.81	15.00
197 ALA CA	5.38	19.48	74.52	15.00
197 ALA CB	6.32	18.63	73.67	15.00
197 ALA C	6.01	19.71	75.90	15.00
197 ALA O	6.93	20.50	76.02	15.00
198 ARG N	5.56	19.01	76.94	15.00
198 ARG CA	6.13	19.21	78.27	15.00
198 ARG CB	5.05	19.61	79.26	15.00
198 ARG CG	5.46	19.52	80.76	15.00
198 ARG CD	4.45	20.21	81.65	15.00
198 ARG NE	3.20	19.48	81.76	15.00
198 ARG CZ	3.00	18.51	82.64	15.00
198 ARG NH1	3.99	18.18	83.47	15.00
198 ARG NH2	1.80	17.95	82.78	15.00
198 ARG C	6.82	17.93	78.72	15.00
198 ARG O	6.19	16.88	78.82	15.00
199 ASN N	8.13	18.02	78.90	15.00
199 ASN CA	8.99	16.89	79.34	15.00
199 ASN CB	8.28	15.93	80.33	15.00
199 ASN CG	8.26	16.47	81.77	15.00
199 ASN OD1	7.22	16.83	82.31	15.00
199 ASN ND2	9.45	16.55	82.38	15.00
199 ASN C	9.79	16.12	78.28	15.00
199 ASN O	10.49	15.17	78.61	15.00
200 LYS N	9.77	16.62	77.05	15.00
200 LYS CA	10.56	16.06	75.94	15.00
200 LYS CB	9.83	16.23	74.61	15.00
200 LYS CG	8.82	15.14	74.28	15.00
200 LYS CD	7.48	15.29	74.99	15.00
200 LYS CE	6.27	15.00	74.07	15.00
200 LYS NZ	6.29	13.60	73.43	15.00
200 LYS C	11.87	16.86	75.92	15.00
200 LYS O	12.15	17.61	74.99	15.00
201 ASN N	12.64	16.70	76.99	15.00
201 ASN CA	13.91	17.41	77.22	15.00

TABLE X

201 ASN CB	15.14	16.71	76.60	15.00
201 ASN CG	15.48	15.43	77.29	15.00
201 ASN OD1	15.33	14.36	76.70	15.00
201 ASN ND2	15.91	15.52	78.56	15.00
201 ASN C	13.91	18.86	76.81	15.00
201 ASN O	14.74	19.28	76.01	15.00
202 ASN N	13.02	19.62	77.41	15.00
202 ASN CA	12.87	21.05	77.17	15.00
202 ASN CB	13.98	21.82	77.88	15.00
202 ASN CG	13.66	23.27	78.07	15.00
202 ASN OD1	12.53	23.63	78.38	15.00
202 ASN ND2	14.63	24.12	77.83	15.00
202 ASN C	12.73	21.47	75.69	15.00
202 ASN O	13.48	22.28	75.16	15.00
203 ALA N	11.66	21.00	75.05	15.00
203 ALA H	11.06	20.52	75.65	15.00
203 ALA CA	11.34	21.22	73.64	15.00
203 ALA CB	10.03	20.53	73.27	15.00
203 ALA C	11.16	22.72	73.38	15.00
203 ALA O	10.25	23.38	73.78	15.00
204 CYS N	11.98	23.21	72.42	15.00
204 CYS CA	12.00	24.60	72.00	15.00
204 CYS C	12.56	25.58	73.01	15.00
204 CYS O	12.50	26.79	72.81	15.00
204 CYS CB	10.64	25.06	71.56	15.00
204 CYS SG	10.05	24.34	69.96	15.00
205 GLY N	13.03	25.04	74.13	15.00
205 GLY CA	13.63	25.86	75.14	15.00
205 GLY C	12.69	26.61	76.01	15.00
205 GLY O	13.03	27.59	76.63	15.00
206 ILE N	11.50	26.08	76.12	15.00
206 ILE CA	10.47	26.69	76.92	15.00
206 ILE CB	9.30	25.69	77.08	15.00
206 ILE CG2	9.78	24.44	77.78	15.00
206 ILE CG1	8.15	26.33	77.87	15.00
206 ILE CD1	7.20	27.12	77.00	15.00
206 ILE C	10.95	27.11	78.33	15.00
206 ILE O	10.50	28.12	78.86	15.00
207 ALA N	11.85	26.34	78.95	15.00
207 ALA CA	12.32	26.67	80.30	15.00
207 ALA CB	12.30	25.45	81.18	15.00
207 ALA C	13.68	27.35	80.43	15.00
207 ALA O	14.20	27.46	81.56	15.00

TABLE X

208 ASN N	14.21	27.84	79.31	15.00
208 ASN CA	15.51	28.52	79.26	15.00
208 ASN CB	16.13	28.39	77.88	15.00
208 ASN CG	16.75	27.01	77.59	15.00
208 ASN OD1	16.26	25.96	78.00	15.00
208 ASN ND2	17.86	27.03	76.88	15.00
208 ASN C	15.37	30.02	79.55	15.00
208 ASN O	16.37	30.73	79.73	15.00
209 LEU N	14.16	30.55	79.48	15.00
209 LEU CA	13.97	31.98	79.73	15.00
209 LEU CB	14.05	32.79	78.43	15.00
209 LEU CG	14.45	34.26	78.52	15.00
209 LEU CD1	15.95	34.30	78.78	15.00
209 LEU CD2	14.12	35.06	77.23	15.00
209 LEU C	12.71	32.35	80.51	15.00
209 LEU O	12.13	33.44	80.31	15.00
210 ALA N	12.37	31.55	81.52	15.00
210 ALA H	12.79	30.67	81.51	15.00
210 ALA CA	11.14	31.81	82.27	15.00
210 ALA CB	10.61	30.53	82.92	15.00
210 ALA C	11.43	32.81	83.41	15.00
210 ALA O	12.41	32.78	84.11	15.00
211 SER N	10.44	33.74	83.58	15.00
211 SER CA	10.44	34.68	84.69	15.00
211 SER CB	11.25	35.95	84.38	15.00
211 SER OG	10.66	36.74	83.37	15.00
211 SER C	8.97	35.02	85.03	15.00
211 SER O	8.07	34.77	84.22	15.00
212 PHE N	8.74	35.50	86.25	15.00
212 PHE CA	7.44	35.96	86.75	15.00
212 PHE CB	6.68	34.87	87.53	15.00
212 PHE CG	7.43	34.30	88.72	15.00
212 PHE CD1	8.34	33.31	88.54	15.00
212 PHE CD2	7.26	34.79	90.01	15.00
212 PHE CE1	9.08	32.83	89.64	15.00
212 PHE CE2	8.00	34.30	91.08	15.00
212 PHE CZ	8.90	33.33	90.90	15.00
212 PHE C	7.65	37.23	87.63	15.00
212 PHE O	8.64	37.35	88.34	15.00
213 PRO N	6.79	38.23	87.46	15.00
213 PRO CD	5.64	38.27	86.55	15.00
213 PRO CA	6.88	39.49	88.23	15.00
213 PRO CB	6.03	40.48	87.41	15.00

TABLE X

213	PRO CG	4.96	39.59	87.00	15.00
213	PRO C	6.30	39.32	89.66	15.00
213	PRO O	5.25	38.68	89.88	15.00
214	LYS N	6.99	39.82	90.67	15.00
214	LYS CA	6.40	39.71	92.01	15.00
214	LYS CB	7.46	39.54	93.11	15.00
214	LYS CG	8.31	38.28	92.90	15.00
214	LYS CD	8.81	37.72	94.19	15.00
214	LYS CE	9.63	38.73	94.95	15.00
214	LYS NZ	10.60	39.41	94.05	15.00
214	LYS C	5.57	40.96	92.27	15.00
214	LYS O	5.99	42.07	91.94	15.00
215	MET N	4.33	40.78	92.72	15.00
215	MET CA	3.47	41.93	92.99	15.00
215	MET CB	2.11	41.74	92.32	15.00
215	MET CG	1.57	43.08	91.85	15.00
215	MET SD	0.31	43.10	90.56	15.00
215	MET CE	-1.09	43.67	91.53	15.00
215	MET C	3.31	42.16	94.50	15.00
215	MET OT1	3.48	41.21	95.29	15.00
215	MET OT2	3.17	43.33	94.89	15.00
216	HOH OH2	8.87	46.84	97.48	15.00
217	HOH OH2	-2.18	37.97	73.56	15.00
218	HOH OH2	1.71	36.04	75.21	15.00
219	HOH OH2	9.44	52.65	61.91	15.00
220	HOH OH2	0.80	56.90	67.17	15.00
221	HOH OH2	-2.51	36.41	82.35	15.00
222	HOH OH2	17.40	43.23	83.47	15.00
223	HOH OH2	-1.57	52.44	64.46	15.00
224	HOH OH2	12.41	35.91	80.62	15.00
225	HOH OH2	11.65	62.93	58.36	15.00
226	HOH OH2	11.38	48.93	74.41	15.00
227	HOH OH2	5.00	12.95	78.69	15.00
228	HOH OH2	4.86	15.66	86.17	15.00
229	HOH OH2	-9.01	32.96	72.96	15.00
230	HOH OH2	14.02	19.79	82.02	15.00
231	HOH OH2	18.09	36.59	88.86	15.00
232	HOH OH2	0.22	37.62	76.69	15.00
233	HOH OH2	3.45	36.52	73.19	15.00
234	HOH OH2	13.53	38.17	80.00	15.00
235	HOH OH2	-15.93	48.59	69.63	15.00
236	HOH OH2	-5.38	44.85	97.00	15.00
237	HOH OH2	-7.89	45.15	89.13	15.00

TABLE X

238 HOH OH2	2.43	19.39	65.70	15.00
239 HOH OH2	7.43	21.65	71.07	15.00
240 HOH OH2	2.41	16.41	85.78	15.00
241 HOH OH2	-0.33	36.99	59.82	15.00
242 HOH OH2	-7.54	26.54	72.89	15.00
243 HOH OH2	-3.03	44.85	65.86	15.00
244 HOH OH2	0.80	35.69	86.28	15.00
245 HOH OH2	-9.57	36.85	95.54	15.00
246 HOH OH2	-1.06	62.37	83.93	15.00
247 HOH OH2	7.72	62.09	69.81	15.00
248 HOH OH2	4.95	60.85	80.90	15.00
249 HOH OH2	14.51	30.92	83.13	15.00
250 HOH OH2	-1.50	28.47	63.31	15.00
251 HOH OH2	15.32	22.32	71.31	15.00
252 HOH OH2	-1.00	14.71	55.75	15.00
253 HOH OH2	6.77	18.87	84.05	15.00
254 HOH OH2	-9.65	32.88	79.27	15.00
255 HOH OH2	-2.32	34.26	69.09	15.00
256 HOH OH2	-11.12	32.20	64.94	15.00
257 HOH OH2	-3.80	45.19	72.07	15.00
258 HOH OH2	-7.43	38.35	65.10	15.00
259 HOH OH2	1.41	46.77	63.08	15.00
260 HOH OH2	-3.18	37.41	80.05	15.00
261 HOH OH2	7.12	59.13	81.53	15.00
262 HOH OH2	9.18	59.65	79.58	15.00
263 HOH OH2	8.43	57.49	83.56	15.00
264 HOH OH2	22.06	33.25	80.24	15.00
265 HOH OH2	20.66	27.84	95.17	15.00
266 HOH OH2	17.09	49.08	84.72	15.00
267 HOH OH2	12.06	54.25	84.82	15.00
268 HOH OH2	9.93	50.78	92.92	15.00
269 HOH OH2	13.59	41.50	91.19	15.00
270 HOH OH2	11.18	49.64	64.47	15.00
271 HOH OH2	12.14	55.71	75.81	15.00
272 HOH OH2	9.07	26.37	66.15	15.00
273 HOH OH2	24.27	24.31	64.11	15.00
274 HOH OH2	18.35	21.16	79.19	15.00
275 HOH OH2	20.62	28.49	61.87	15.00
276 HOH OH2	13.58	15.19	72.83	15.00
277 HOH OH2	9.33	19.74	77.14	15.00

TABLE XI

Table of angles between atoms of the inhibitor and protein for all protein atoms within 5 Ångstroms of the inhibitor 3(S)-3-[(N-benzyloxycarbonyl)-L-leucinyl]amino-5-methyl-1-(1-propoxy)-2-hexanone.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
242OH2	25C1	18OD1	69.66	242OH2	25C1	18ND2	48.33
242OH2	25C1	184O	82.25	242OH2	25C1	18CG	62.66
242OH2	25C1	184C	92.20	18OD1	25C1	184CA	78.01
18OD1	25C1	18ND2	33.84	18OD1	25C1	184O	82.68
18OD1	25C1	184CD1	97.11	18OD1	25C1	18CG	16.91
18OD1	25C1	184C	73.04	18OD1	25C1	20O	60.56
184CB	25C1	184CA	23.31	184CB	25C1	18ND2	93.14
184CB	25C1	184O	42.27	184CB	25C1	184CG	22.32
184CB	25C1	184CD1	38.40	184CB	25C1	18CG	92.58
184CB	25C1	184C	36.61	184CB	25C1	184CD2	32.79
184CB	25C1	184NE1	49.18	184CA	25C1	18ND2	72.65
184CA	25C1	184O	35.91	184CA	25C1	184CG	38.24
184CA	25C1	184CD1	44.79	184CA	25C1	18CG	69.61
184CA	25C1	184C	21.48	184CA	25C1	184CD2	52.43
184CA	25C1	184NE1	58.86	18ND2	25C1	184O	58.28
18ND2	25C1	18CG	18.49	18ND2	25C1	184C	56.82
18ND2	25C1	20O	92.88	184O	25C1	184CG	64.55
184O	25C1	184CD1	78.02	184O	25C1	18CG	67.10
184O	25C1	184C	17.17	184O	25C1	184CD2	73.76
184O	25C1	184NE1	90.68	184CG	25C1	184CD1	19.59
184CG	25C1	184C	56.91	184CG	25C1	184CD2	15.07
184CG	25C1	184NE1	27.32	184CD1	25C1	18CG	99.42
184CD1	25C1	184C	66.13	184CD1	25C1	184CD2	27.32
184CD1	25C1	184NE1	14.36	184CD1	25C1	20O	86.22
18CG	25C1	184C	59.85	18CG	25C1	20O	77.46
184C	25C1	184CD2	69.30	184C	25C1	184NE1	80.01
184CD2	25C1	184NE1	26.78	184NE1	25C1	20O	80.98
18OD1	25C2	184CA	93.13	18OD1	25C2	18CG	18.16
18OD1	25C2	20N	42.62	18OD1	25C2	18ND2	35.44
18OD1	25C2	242OH2	68.83	18OD1	25C2	20O	79.33
18OD1	25C2	183O	73.73	18OD1	25C2	184C	80.63
18OD1	25C2	19CG	85.64	18OD1	25C2	20CA	45.72
18OD1	25C2	19N	47.90	18OD1	25C2	184O	85.52
18OD1	25C2	20C	65.28	18OD1	25C2	184N	90.71
18OD1	25C2	19C	49.49	18OD1	25C2	18CB	22.83

TABLE XI

18OD1	25C2	183C	82.72	18OD1	25C2	18CA	34.96
18OD1	25C2	18C	34.23	18OD1	25C2	19CA	54.26
184CD1	25C2	184CA	49.90	184CD1	25C2	184CB	40.27
184CD1	25C2	184CG	20.32	184CD1	25C2	183O	55.01
184CD1	25C2	184C	70.22	184CD1	25C2	19CG	61.53
184CD1	25C2	19N	85.18	184CD1	25C2	184O	78.11
184CD1	25C2	184NE1	15.62	184CD1	25C2	184N	44.48
184CD1	25C2	183C	47.20	184CD1	25C2	18CA	94.36
184CD1	25C2	18C	95.90	184CD1	25C2	184CD2	23.77
184CD1	25C2	19CA	87.00	184CA	25C2	18CG	78.59
184CA	25C2	18ND2	76.16	184CA	25C2	184CB	23.25
184CA	25C2	184CG	39.72	184CA	25C2	183O	40.92
184CA	25C2	184C	20.77	184CA	25C2	19CG	86.38
184CA	25C2	19N	76.16	184CA	25C2	184O	33.25
184CA	25C2	184NE1	65.31	184CA	25C2	184N	13.46
184CA	25C2	18CB	70.34	184CA	25C2	183C	28.93
184CA	25C2	18CA	61.99	184CA	25C2	18C	75.30
184CA	25C2	184CD2	51.97	184CA	25C2	19CA	89.58
18CG	25C2	20N	59.81	18CG	25C2	18ND2	20.07
18CG	25C2	184CB	99.39	18CG	25C2	242OH2	62.04
18CG	25C2	20O	97.48	18CG	25C2	183O	69.32
18CG	25C2	184C	63.66	18CG	25C2	19CG	95.51
18CG	25C2	20CA	63.78	18CG	25C2	19N	54.69
18CG	25C2	184O	67.41	18CG	25C2	20C	83.28
18CG	25C2	184N	79.10	18CG	25C2	19C	65.07
18CG	25C2	18CB	12.54	18CG	25C2	183C	75.08
18CG	25C2	18CA	30.58	18CG	25C2	18C	39.48
18CG	25C2	19CA	65.54	20N	25C2	18ND2	78.04
20N	25C2	20O	42.02	20N	25C2	183O	74.98
20N	25C2	19CG	52.80	20N	25C2	20CA	19.88
20N	25C2	19N	37.71	20N	25C2	20C	32.71
20N	25C2	19C	11.44	20N	25C2	18CB	58.04
20N	25C2	183C	87.83	20N	25C2	18CA	55.70
20N	25C2	18C	39.13	20N	25C2	19CA	28.06
18ND2	25C2	184CB	92.26	18ND2	25C2	242OH2	45.09
18ND2	25C2	183O	80.83	18ND2	25C2	184C	57.03
18ND2	25C2	20CA	77.75	18ND2	25C2	19N	73.94
18ND2	25C2	184O	55.05	18ND2	25C2	20C	96.02
18ND2	25C2	184N	81.33	18ND2	25C2	19C	84.52
18ND2	25C2	18CB	29.48	18ND2	25C2	183C	82.74
18ND2	25C2	18CA	46.57	18ND2	25C2	18C	58.80
18ND2	25C2	19CA	85.56	184CB	25C2	184CG	22.40
184CB	25C2	183O	59.35	184CB	25C2	184C	36.03
184CB	25C2	19CG	94.64	184CB	25C2	19N	96.61

TABLE XI

184CB	25C2	184O	38.77	184CB	25C2	184NE1	52.96
184CB	25C2	184N	31.46	184CB	25C2	18CB	92.63
184CB	25C2	183C	46.49	184CB	25C2	18CA	85.24
184CB	25C2	18C	97.95	184CB	25C2	184CD2	31.97
242OH2	25C2	184C	81.46	242OH2	25C2	20CA	87.88
242OH2	25C2	184O	68.50	242OH2	25C2	20C	95.83
242OH2	25C2	18CB	73.69	242OH2	25C2	18CA	91.46
184CG	25C2	183O	61.89	184CG	25C2	184C	57.17
184CG	25C2	19CG	81.07	184CG	25C2	19N	97.59
184CG	25C2	184O	61.14	184CG	25C2	184NE1	30.80
184CG	25C2	184N	40.66	184CG	25C2	183C	50.54
184CG	25C2	18CA	97.12	184CG	25C2	184CD2	12.85
200	25C2	19CG	59.65	200	25C2	20CA	33.80
200	25C2	19N	73.93	200	25C2	184NE1	98.68
200	25C2	20C	15.00	200	25C2	19C	44.20
200	25C2	18CB	98.94	200	25C2	18CA	97.51
200	25C2	18C	80.19	200	25C2	19CA	58.60
183O	25C2	184C	52.11	183O	25C2	19CG	50.15
183O	25C2	20CA	94.61	183O	25C2	19N	37.44
183O	25C2	184O	68.46	183O	25C2	184NE1	67.20
183O	25C2	184N	28.51	183O	25C2	19C	66.39
183O	25C2	18CB	56.86	183O	25C2	183C	12.86
183O	25C2	18CA	39.61	183O	25C2	18C	42.74
183O	25C2	184CD2	73.55	183O	25C2	19CA	48.97
184C	25C2	19N	79.88	184C	25C2	184O	16.37
184C	25C2	184NE1	85.33	184C	25C2	184N	31.43
184C	25C2	18CB	58.56	184C	25C2	183C	43.26
184C	25C2	18CA	56.66	184C	25C2	18C	73.56
184C	25C2	184CD2	67.95	184C	25C2	19CA	95.56
19CG	25C2	20CA	68.54	19CG	25C2	19N	41.00
19CG	25C2	184NE1	59.71	19CG	25C2	20C	65.93
19CG	25C2	184N	72.99	19CG	25C2	19C	41.61
19CG	25C2	18CB	85.55	19CG	25C2	183C	58.81
19CG	25C2	18CA	69.73	19CG	25C2	18C	56.16
19CG	25C2	184CD2	84.49	19CG	25C2	19CA	31.40
20CA	25C2	19N	57.18	20CA	25C2	20C	19.60
20CA	25C2	19C	30.27	20CA	25C2	18CB	66.65
20CA	25C2	18CA	70.02	20CA	25C2	18C	55.87
20CA	25C2	19CA	47.75	19N	25C2	184O	94.75
19N	25C2	184NE1	91.69	19N	25C2	20C	69.08
19N	25C2	184N	65.26	19N	25C2	19C	30.47
19N	25C2	18CB	44.60	19N	25C2	183C	50.23
19N	25C2	18CA	30.19	19N	25C2	18C	15.21
19N	25C2	19CA	16.11	184O	25C2	184NE1	91.68

TABLE XI

1840	25C2	184N	45.89	1840	25C2	18CB	65.91
1840	25C2	183C	59.15	1840	25C2	18CA	68.65
1840	25C2	18C	86.43	1840	25C2	184CD2	69.23
184NE1	25C2	184N	60.01	184NE1	25C2	183C	61.27
184NE1	25C2	184CD2	26.96	184NE1	25C2	19CA	89.32
20C	25C2	19C	38.71	20C	25C2	18CB	86.12
20C	25C2	18CA	87.75	20C	25C2	18C	71.80
20C	25C2	19CA	55.73	184N	25C2	19C	94.86
184N	25C2	18CB	68.81	184N	25C2	183C	15.92
184N	25C2	18CA	56.71	184N	25C2	18C	67.03
184N	25C2	184CD2	53.50	184N	25C2	19CA	77.48
19C	25C2	18CB	60.71	19C	25C2	183C	79.19
19C	25C2	18CA	54.22	19C	25C2	18C	36.38
19C	25C2	19CA	17.76	18CB	25C2	183C	63.21
18CB	25C2	18CA	18.13	18CB	25C2	18C	29.64
18CB	25C2	19CA	57.42	183C	25C2	18CA	47.76
183C	25C2	18C	54.26	183C	25C2	184CD2	62.80
183C	25C2	19CA	61.67	18CA	25C2	18C	17.97
18CA	25C2	19CA	45.40	18C	25C2	19CA	28.26
200	25C3	19CG	77.70	200	25C3	20N	48.86
200	25C3	18OD1	82.41	200	25C3	20C	15.02
200	25C3	20CA	36.52	200	25C3	19CD	82.71
200	25C3	19C	49.69	200	25C3	19N	81.60
200	25C3	19CB	69.52	200	25C3	18CG	93.56
200	25C3	19OE1	97.10	200	25C3	19CA	66.55
184CD1	25C3	19CG	70.95	184CD1	25C3	184NE1	20.32
184CD1	25C3	184CG	17.18	184CD1	25C3	19CD	63.15
184CD1	25C3	19N	84.37	184CD1	25C3	184CA	41.74
184CD1	25C3	183O	51.08	184CD1	25C3	19CB	82.21
184CD1	25C3	184CB	33.05	184CD1	25C3	18CG	99.94
184CD1	25C3	19OE1	48.60	184CD1	25C3	19CA	92.55
184CD1	25C3	184CE2	24.46	19CG	25C3	20N	60.87
19CG	25C3	18OD1	86.79	19CG	25C3	20C	80.83
19CG	25C3	184NE1	70.80	19CG	25C3	20CA	78.71
19CG	25C3	184CG	86.74	19CG	25C3	19CD	19.15
19CG	25C3	19C	46.56	19CG	25C3	19N	42.15
19CG	25C3	184CA	83.50	19CG	25C3	183O	50.42
19CG	25C3	19CB	14.34	19CG	25C3	184CB	93.55
19CG	25C3	18CG	90.03	19CG	25C3	19OE1	29.89
19CG	25C3	19CA	32.74	19CG	25C3	184CE2	83.95
20N	25C3	18OD1	40.95	20N	25C3	20C	38.02
20N	25C3	20CA	21.15	20N	25C3	19CD	78.19
20N	25C3	19C	14.72	20N	25C3	19N	36.90
20N	25C3	184CA	98.63	20N	25C3	183O	71.83

TABLE XI

20N	25C3	19CB	46.57	20N	25C3	18CG	51.19
20N	25C3	19OE1	90.75	20N	25C3	19CA	30.28
20N	25C3	242OH2	86.06	18OD1	25C3	20C	67.75
18OD1	25C3	20CA	45.89	18OD1	25C3	19C	52.30
18OD1	25C3	19N	45.18	18OD1	25C3	184CA	70.04
18OD1	25C3	183O	62.55	18OD1	25C3	19CB	74.34
18OD1	25C3	184CB	86.92	18OD1	25C3	18CG	11.19
18OD1	25C3	19CA	55.77	18OD1	25C3	242OH2	51.35
20C	25C3	20CA	22.11	20C	25C3	19CD	90.19
20C	25C3	19C	43.18	20C	25C3	19N	73.89
20C	25C3	19CB	69.80	20C	25C3	18CG	78.83
20C	25C3	19CA	61.77	20C	25C3	242OH2	89.06
184NE1	25C3	184CG	32.04	184NE1	25C3	19CD	56.99
184NE1	25C3	19N	96.67	184NE1	25C3	184CA	61.92
184NE1	25C3	183O	67.54	184NE1	25C3	19CB	84.48
184NE1	25C3	184CB	50.65	184NE1	25C3	19OE1	42.30
184NE1	25C3	19CA	99.57	184NE1	25C3	184CE2	13.16
20CA	25C3	19CD	93.68	20CA	25C3	19C	32.85
20CA	25C3	19N	57.68	20CA	25C3	183O	91.89
20CA	25C3	19CB	64.99	20CA	25C3	18CG	57.06
20CA	25C3	19CA	50.80	20CA	25C3	242OH2	76.89
184CG	25C3	19CD	80.27	184CG	25C3	19N	91.72
184CG	25C3	184CA	34.06	184CG	25C3	183O	56.45
184CG	25C3	19CB	96.63	184CG	25C3	184CB	18.84
184CG	25C3	18CG	93.58	184CG	25C3	19OE1	65.78
184CG	25C3	184CE2	28.26	184CG	25C3	242OH2	94.95
19CD	25C3	19C	63.50	19CD	25C3	19N	60.85
19CD	25C3	184CA	88.20	19CD	25C3	183O	60.91
19CD	25C3	19CB	32.82	19CD	25C3	184CB	92.35
19CD	25C3	19OE1	14.96	19CD	25C3	19CA	51.66
19CD	25C3	184CE2	69.81	19C	25C3	19N	31.91
19C	25C3	184CA	98.36	19C	25C3	183O	66.62
19C	25C3	19CB	32.43	19C	25C3	18CG	61.26
19C	25C3	19OE1	76.35	19C	25C3	19CA	18.84
19N	25C3	184CA	66.70	19N	25C3	183O	35.29
19N	25C3	19CB	31.75	19N	25C3	184CB	85.03
19N	25C3	18CG	47.94	19N	25C3	19OE1	67.18
19N	25C3	19CA	17.97	19N	25C3	242OH2	95.18
184CA	25C3	183O	35.33	184CA	25C3	19CB	86.05
184CA	25C3	184CB	19.26	184CA	25C3	18CG	59.77
184CA	25C3	19OE1	78.16	184CA	25C3	19CA	83.25
184CA	25C3	184CE2	61.84	184CA	25C3	242OH2	75.15
183O	25C3	19CB	50.84	183O	25C3	184CB	51.32
183O	25C3	18CG	57.48	183O	25C3	19OE1	57.08

TABLE XI

1830	25C3	19CA	49.31	1830	25C3	184CE2	75.42
1830	25C3	242OH2	96.01	19CB	25C3	184CB	99.69
19CB	25C3	18CG	79.10	19CB	25C3	19OE1	44.22
19CB	25C3	19CA	18.92	19CB	25C3	184CE2	97.58
184CB	25C3	18CG	76.03	184CB	25C3	19OE1	79.22
184CB	25C3	184CE2	46.73	184CB	25C3	242OH2	78.05
18CG	25C3	19CA	61.53	18CG	25C3	242OH2	47.27
19OE1	25C3	19CA	62.05	19OE1	25C3	184CE2	55.29
200	25C4	20C	10.43	200	25C4	19CG	62.30
200	25C4	20N	35.25	200	25C4	20CA	26.32
200	25C4	19CD	71.57	200	25C4	21NE2	50.82
200	25C4	18OD1	61.89	184CD1	25C4	184NE1	20.27
184CD1	25C4	19CG	57.56	184CD1	25C4	184CG	16.41
184CD1	25C4	184CE2	28.68	184CD1	25C4	20N	90.35
184CD1	25C4	19CD	54.84	184CD1	25C4	18OD1	81.65
184CD1	25C4	184CD2	25.56	184NE1	25C4	19CG	61.65
184NE1	25C4	184CG	29.79	184NE1	25C4	184CE2	15.87
184NE1	25C4	19CD	51.78	184NE1	25C4	184CD2	25.93
20C	25C4	19CG	66.50	20C	25C4	20N	31.03
20C	25C4	20CA	17.90	20C	25C4	19CD	78.21
20C	25C4	21NE2	44.60	20C	25C4	18OD1	53.90
19CG	25C4	184CG	72.66	19CG	25C4	184CE2	77.52
19CG	25C4	20N	46.19	19CG	25C4	20CA	61.94
19CG	25C4	19CD	18.17	19CG	25C4	18OD1	63.67
19CG	25C4	184CD2	82.38	184CG	25C4	184CE2	28.98
184CG	25C4	20N	98.65	184CG	25C4	19CD	71.23
184CG	25C4	18OD1	82.35	184CG	25C4	184CD2	16.48
184CE2	25C4	19CD	67.12	184CE2	25C4	184CD2	16.42
20N	25C4	20CA	17.47	20N	25C4	19CD	63.14
20N	25C4	21NE2	68.18	20N	25C4	18OD1	30.69
20CA	25C4	19CD	77.50	20CA	25C4	21NE2	50.79
20CA	25C4	18OD1	36.03	19CD	25C4	18OD1	81.70
19CD	25C4	184CD2	76.27	21NE2	25C4	18OD1	71.09
18OD1	25C4	184CD2	98.63	184CD1	25C5	200	89.99
184CD1	25C5	184NE1	17.97	184CD1	25C5	184CG	17.29
184CD1	25C5	184CE2	27.88	184CD1	25C5	242OH2	99.26
184CD1	25C5	184CD2	27.37	200	25C5	184NE1	92.08
200	25C5	242OH2	86.50	200	25C5	21NE2	47.88
184NE1	25C5	184CG	28.79	184NE1	25C5	184CE2	16.62
184NE1	25C5	184CD2	27.40	184CG	25C5	184CE2	28.30
184CG	25C5	242OH2	92.08	184CG	25C5	184CD2	17.13
184CE2	25C5	184CD2	16.84	242OH2	25C5	21NE2	65.12
242OH2	25C6	184CB	96.30	242OH2	25C6	184CA	83.88
242OH2	25C6	18OD1	51.77	242OH2	25C6	184O	63.15

TABLE XI

184CG	25C6	184CD1	17.92	184CG	25C6	184CB	19.89
184CG	25C6	184CD2	17.11	184CG	25C6	184NE1	27.45
184CG	25C6	184CA	31.62	184CG	25C6	18OD1	84.34
184CG	25C6	184O	53.51	184CD1	25C6	184CB	33.90
184CD1	25C6	184CD2	27.70	184CD1	25C6	184NE1	16.02
184CD1	25C6	184CA	37.26	184CD1	25C6	18OD1	76.75
184CD1	25C6	184O	64.28	184CB	25C6	184CD2	32.92
184CB	25C6	184NE1	46.79	184CB	25C6	184CA	18.16
184CB	25C6	18OD1	76.20	184CB	25C6	184O	33.78
184CD2	25C6	184NE1	26.79	184CD2	25C6	184CA	47.98
184CD2	25C6	184O	65.87	184NE1	25C6	184CA	53.03
184NE1	25C6	18OD1	88.79	184NE1	25C6	184O	79.21
184CA	25C6	18OD1	58.04	184CA	25C6	184O	28.15
18OD1	25C6	184O	61.50	200	25C7	20C	4.43
200	25C7	19CG	62.28	200	25C7	19CD	77.38
200	25C7	19NE2	74.82	200	25C7	19OE1	90.67
184NE1	25C7	19CG	59.54	184NE1	25C7	19CD	53.46
184NE1	25C7	184CD1	17.49	184NE1	25C7	19NE2	66.80
184NE1	25C7	19OE1	40.08	184NE1	25C7	184CE2	14.60
20C	25C7	19CG	65.46	20C	25C7	19CD	81.18
20C	25C7	19NE2	79.11	20C	25C7	19OE1	94.22
19CG	25C7	19CD	19.72	19CG	25C7	184CD1	52.93
19CG	25C7	19NE2	30.67	19CG	25C7	19OE1	29.47
19CG	25C7	184CE2	74.12	19CD	25C7	184CD1	53.97
19CD	25C7	19NE2	16.35	19CD	25C7	19OE1	14.31
19CD	25C7	184CE2	67.37	184CD1	25C7	19NE2	69.74
184CD1	25C7	19OE1	43.73	184CD1	25C7	184CE2	26.87
19NE2	25C7	19OE1	26.90	19NE2	25C7	184CE2	79.58
19OE1	25C7	184CE2	53.50	184NE1	2508	19CD	69.28
184NE1	2508	19NE2	88.26	184NE1	2508	19OE1	52.70
184NE1	2508	19CG	72.15	184NE1	2508	184CD1	18.62
184NE1	2508	184CE2	15.78	184NE1	2508	184CZ2	30.82
19CD	2508	19NE2	21.45	19CD	2508	19OE1	19.40
19CD	2508	19CG	23.73	19CD	2508	200	83.60
19CD	2508	184CD1	65.36	19CD	2508	184CE2	84.12
19CD	2508	220	53.07	19CD	2508	184CZ2	93.15
19NE2	2508	19OE1	35.59	19NE2	2508	19CG	38.13
19NE2	2508	200	82.17	19NE2	2508	184CD1	86.56
19NE2	2508	220	36.04	19OE1	2508	19CG	37.46
19OE1	2508	184CD1	53.61	19OE1	2508	184CE2	66.40
19OE1	2508	220	70.80	19OE1	2508	184CZ2	73.99
19CG	2508	200	63.71	19CG	2508	184CD1	60.70
19CG	2508	184CE2	87.89	19CG	2508	220	54.69
200	2508	220	57.31	184CD1	2508	184CE2	30.67

TABLE XI

184CD1	2508	184CZ2	47.47	184CE2	2508	184CZ2	16.93
19NE2	25C9	184NE1	78.75	19NE2	25C9	19CD	19.52
19NE2	25C9	19OE1	33.07	19NE2	25C9	184CE2	94.10
19NE2	25C9	19CG	30.70	19NE2	25C9	184CD1	73.44
19NE2	25C9	22O	33.46	184NE1	25C9	19CD	59.66
184NE1	25C9	19OE1	47.23	184NE1	25C9	184CE2	16.38
184NE1	25C9	184CZ2	33.08	184NE1	25C9	19CG	58.24
184NE1	25C9	184CD1	12.56	19CD	25C9	19OE1	17.75
19CD	25C9	184CE2	75.46	19CD	25C9	184CZ2	89.07
19CD	25C9	19CG	17.50	19CD	25C9	184CD1	53.92
19CD	25C9	22O	48.71	19OE1	25C9	184CE2	61.55
19OE1	25C9	184CZ2	73.08	19OE1	25C9	19CG	30.61
19OE1	25C9	184CD1	45.28	19OE1	25C9	22O	65.42
184CE2	25C9	184CZ2	17.56	184CE2	25C9	19CG	74.59
184CE2	25C9	184CD1	26.94	184CZ2	25C9	19CG	90.93
184CZ2	25C9	184CD1	44.43	19CG	25C9	184CD1	48.87
19CG	25C9	22O	48.21	184CD1	25C9	22O	97.02
19NE2	25O10	23CA	53.09	19NE2	25O10	19CD	16.71
19NE2	25O10	22O	36.83	19NE2	25O10	23N	57.66
19NE2	25O10	19OE1	28.25	19NE2	25O10	22C	50.13
23CA	25O10	19CD	69.80	23CA	25O10	22O	36.05
23CA	25O10	23N	17.68	23CA	25O10	19OE1	79.02
23CA	25O10	22C	29.83	19CD	25O10	22O	49.55
19CD	25O10	23N	73.42	19CD	25O10	19OE1	15.11
19CD	25O10	22C	63.87	22O	25O10	23N	27.96
22O	25O10	19OE1	63.96	22O	25O10	22C	14.56
23N	25O10	19OE1	85.79	23N	25O10	22C	15.87
19OE1	25O10	22C	77.94	162ND1	25C11	184CZ2	63.39
162ND1	25C11	162CE1	16.78	162ND1	25C11	184NE1	61.01
162ND1	25C11	184CE2	62.72	162ND1	25C11	162CG	15.67
162ND1	25C11	184CH2	68.93	162ND1	25C11	162CB	30.11
184CZ2	25C11	162CE1	53.21	184CZ2	25C11	184NE1	33.69
184CZ2	25C11	184CE2	16.65	184CZ2	25C11	162CG	59.25
184CZ2	25C11	184CH2	12.22	184CZ2	25C11	162CB	70.77
162CE1	25C11	184NE1	44.59	162CE1	25C11	184CE2	48.65
162CE1	25C11	162CG	27.93	162CE1	25C11	184CH2	61.58
162CE1	25C11	162CB	44.93	184NE1	25C11	184CE2	17.24
184NE1	25C11	162CG	67.01	184NE1	25C11	184CH2	45.73
184NE1	25C11	162CB	83.92	184CE2	25C11	162CG	63.63
184CE2	25C11	184CH2	28.52	184CE2	25C11	162CB	78.45
162CG	25C11	184CH2	61.52	162CG	25C11	162CB	17.47
184CH2	25C11	162CB	69.67	138OG	25C15	138CB	12.25
138OG	25C15	138CA	28.90	138OG	25C15	161OD1	38.49
138CB	25C15	138CA	18.42	138CB	25C15	161OD1	45.39

TABLE XI

138CA	25C15	161OD1	48.24	162ND1	25C16	161O	83.50
162ND1	25C16	162CG	18.14	162ND1	25C16	162CE1	16.51
162ND1	25C16	162CB	37.71	162ND1	25C16	25SG	53.12
162ND1	25C16	162CA	45.79	162ND1	25C16	161C	76.59
162ND1	25C16	184CZ2	58.80	162ND1	25C16	25CB	44.47
162ND1	25C16	162N	61.56	162ND1	25C16	19OE1	54.44
161O	25C16	162CG	73.87	161O	25C16	162CE1	99.61
161O	25C16	162CB	55.47	161O	25C16	25SG	68.22
161O	25C16	162CA	38.54	161O	25C16	161C	12.03
161O	25C16	25CB	87.95	161O	25C16	162N	25.97
162CG	25C16	162CE1	32.06	162CG	25C16	162CB	21.17
162CG	25C16	25SG	64.52	162CG	25C16	162CA	35.58
162CG	25C16	161C	64.63	162CG	25C16	184CZ2	58.11
162CG	25C16	25CB	60.75	162CG	25C16	162N	48.98
162CG	25C16	19OE1	71.80	162CE1	25C16	162CB	53.00
162CE1	25C16	25SG	57.54	162CE1	25C16	162CA	62.27
162CE1	25C16	161C	93.08	162CE1	25C16	184CZ2	50.19
162CE1	25C16	25CB	42.26	162CE1	25C16	162N	78.06
162CE1	25C16	19OE1	40.00	162CB	25C16	25SG	70.05
162CB	25C16	162CA	20.87	162CB	25C16	161C	44.96
162CB	25C16	184CZ2	71.73	162CB	25C16	25CB	73.86
162CB	25C16	162N	29.56	162CB	25C16	19OE1	92.15
25SG	25C16	162CA	56.57	25SG	25C16	161C	72.16
25SG	25C16	25CB	21.35	25SG	25C16	162N	67.66
25SG	25C16	19OE1	58.28	162CA	25C16	161C	30.81
162CA	25C16	184CZ2	91.78	162CA	25C16	25CB	67.26
162CA	25C16	162N	16.41	162CA	25C16	19OE1	95.96
161C	25C16	25CB	89.77	161C	25C16	162N	15.65
184CZ2	25C16	25CB	89.70	184CZ2	25C16	19OE1	64.53
25CB	25C16	162N	81.65	25CB	25C16	19OE1	37.30
162ND1	25O17	162CB	53.19	162ND1	25O17	162CG	26.33
162ND1	25O17	162CA	63.48	162ND1	25O17	162N	85.18
162ND1	25O17	162CE1	12.84	162ND1	25O17	25SG	56.41
162ND1	25O17	162CD2	24.16	162ND1	25O17	162C	54.50
162ND1	25O17	162NE2	14.17	162ND1	25O17	184CZ2	59.71
162ND1	25O17	163N	47.86	162ND1	25O17	25CB	41.51
162CB	25O17	161O	76.56	162CB	25O17	162CG	28.45
162CB	25O17	162CA	28.85	162CB	25O17	161C	60.68
162CB	25O17	162N	40.36	162CB	25O17	162CE1	64.12
162CB	25O17	25SG	83.81	162CB	25O17	161OD1	58.91
162CB	25O17	162CD2	36.23	162CB	25O17	162C	31.62
162CB	25O17	162NE2	52.83	162CB	25O17	184CZ2	81.36
162CB	25O17	163N	44.40	162CB	25O17	25CB	83.22
162CB	25O17	161CA	66.51	162CB	25O17	161CB	74.63

TABLE XI

1610	25017 162CA	52.04	1610	25017 161C	18.10
1610	25017 162N	36.49	1610	25017 25SG	77.20
1610	25017 161OD1	60.19	1610	25017 162C	58.32
1610	25017 163N	63.78	1610	25017 25CB	97.03
1610	25017 161CA	21.34	1610	25017 161CB	35.39
162CG	25017 162CA	48.03	162CG	25017 161C	86.77
162CG	25017 162N	66.31	162CG	25017 162CE1	35.94
162CG	25017 25SG	73.55	162CG	25017 161OD1	84.63
162CG	25017 162CD2	9.57	162CG	25017 162C	43.30
162CG	25017 162NE2	24.46	162CG	25017 184CZ2	61.90
162CG	25017 163N	46.12	162CG	25017 25CB	64.34
162CG	25017 161CA	94.08	162CA	25017 161C	40.53
162CA	25017 162N	22.22	162CA	25017 162CE1	76.31
162CA	25017 25SG	66.07	162CA	25017 161OD1	63.93
162CA	25017 162CD2	57.57	162CA	25017 162C	11.05
162CA	25017 162NE2	70.12	162CA	25017 163N	26.62
162CA	25017 25CB	74.60	162CA	25017 161CA	50.08
162CA	25017 161CB	64.72	161C	25017 162N	20.53
161C	25017 25SG	84.94	161C	25017 161OD1	45.99
161C	25017 162CD2	95.86	161C	25017 162C	49.50
161C	25017 163N	59.81	161C	25017 161CA	11.07
161C	25017 161CB	28.61	162N	25017 162CE1	97.92
162N	25017 25SG	81.29	162N	25017 161OD1	46.28
162N	25017 162CD2	75.34	162N	25017 162C	32.79
162N	25017 162NE2	90.12	162N	25017 163N	46.59
162N	25017 25CB	94.05	162N	25017 161CA	28.47
162N	25017 161CB	42.50	162CE1	25017 25SG	60.41
162CE1	25017 162CD2	30.63	162CE1	25017 162C	67.29
162CE1	25017 162NE2	14.05	162CE1	25017 184CZ2	50.87
162CE1	25017 163N	59.73	162CE1	25017 25CB	42.09
25SG	25017 162CD2	77.38	25SG	25017 162C	56.56
25SG	25017 162NE2	70.26	25SG	25017 163N	40.80
25SG	25017 25CB	20.52	25SG	25017 161CA	94.97
161OD1	25017 162CD2	88.85	161OD1	25017 162C	74.74
161OD1	25017 163N	90.55	161OD1	25017 161CA	38.88
161OD1	25017 161CB	28.90	162CD2	25017 162C	52.76
162CD2	25017 162NE2	17.33	162CD2	25017 184CZ2	52.52
162CD2	25017 163N	54.44	162CD2	25017 25CB	65.18
162C	25017 162NE2	62.89	162C	25017 163N	16.06
162C	25017 25CB	63.70	162C	25017 161CA	59.72
162C	25017 161CB	75.18	162NE2	25017 184CZ2	46.51
162NE2	25017 163N	59.43	162NE2	25017 25CB	53.98
184CZ2	25017 25CB	88.90	163N	25017 25CB	48.07
163N	25017 161CA	70.75	163N	25017 161CB	87.59

TABLE XI

161CA	25O17	161CB	17.64	25SG	25N18	162ND1	54.05
25SG	25N18	161O	72.12	25SG	25N18	25CB	22.85
25SG	25N18	19NE2	68.04	25SG	25N18	23CA	83.69
25SG	25N18	162CE1	55.83	25SG	25N18	162CA	54.53
25SG	25N18	19OE1	61.94	25SG	25N18	162CG	59.80
25SG	25N18	162CB	64.56	162ND1	25N18	161O	73.75
162ND1	25N18	25CB	47.82	162ND1	25N18	19NE2	80.11
162ND1	25N18	162CE1	14.94	162ND1	25N18	162CA	39.62
162ND1	25N18	19OE1	53.76	162ND1	25N18	162CG	12.62
162ND1	25N18	162CB	29.54	161O	25N18	25CB	91.76
161O	25N18	162CE1	88.51	161O	25N18	162CA	34.27
161O	25N18	162CG	63.44	161O	25N18	162CB	47.06
25CB	25N18	19NE2	48.54	25CB	25N18	23CA	78.61
25CB	25N18	162CE1	42.68	25CB	25N18	162CA	66.30
25CB	25N18	19OE1	39.11	25CB	25N18	162CG	58.13
25CB	25N18	162CB	69.62	19NE2	25N18	23CA	48.32
19NE2	25N18	162CE1	66.29	19NE2	25N18	19OE1	27.62
19NE2	25N18	162CG	92.70	23CA	25N18	19OE1	75.78
162CE1	25N18	162CA	54.27	162CE1	25N18	19OE1	39.27
162CE1	25N18	162CG	26.90	162CE1	25N18	162CB	44.19
162CA	25N18	19OE1	90.56	162CA	25N18	162CG	30.46
162CA	25N18	162CB	17.73	19OE1	25N18	162CG	66.12
19OE1	25N18	162CB	83.30	162CG	25N18	162CB	17.35
25SG	25C19	161O	94.77	25SG	25C19	162ND1	55.31
25SG	25C19	25CB	20.96	25SG	25C19	162CA	63.69
25SG	25C19	161C	89.52	25SG	25C19	23CA	94.30
25SG	25C19	23O	76.83	25SG	25C19	23C	78.19
25SG	25C19	162N	77.13	25SG	25C19	25N	39.34
25SG	25C19	19NE2	66.56	25SG	25C19	163N	35.68
25SG	25C19	162CE1	52.07	25SG	25C19	162CB	68.67
161O	25C19	162ND1	77.82	161O	25C19	162CA	38.27
161O	25C19	161C	6.45	161O	25C19	162N	21.62
161O	25C19	163N	59.92	161O	25C19	162CE1	90.20
161O	25C19	162CB	47.78	162ND1	25C19	25CB	49.17
162ND1	25C19	162CA	42.28	162ND1	25C19	161C	71.68
162ND1	25C19	162N	57.38	162ND1	25C19	25N	77.84
162ND1	25C19	19NE2	72.32	162ND1	25C19	163N	45.25
162ND1	25C19	162CE1	12.42	162ND1	25C19	162CB	30.12
25CB	25C19	162CA	73.53	25CB	25C19	23CA	82.52
25CB	25C19	23O	74.24	25CB	25C19	23C	70.22
25CB	25C19	162N	89.39	25CB	25C19	25N	30.03
25CB	25C19	19NE2	46.97	25CB	25C19	163N	50.32
25CB	25C19	162CE1	41.12	25CB	25C19	162CB	72.32
162CA	25C19	161C	31.82	162CA	25C19	162N	16.65

TABLE XI

162CA	25C19	163N	29.20	162CA	25C19	162CE1	53.97
162CA	25C19	162CB	17.00	161C	25C19	162N	15.17
161C	25C19	163N	54.26	161C	25C19	162CE1	84.02
161C	25C19	162CB	41.75	23CA	25C19	23O	29.88
23CA	25C19	23C	18.55	23CA	25C19	25N	55.13
23CA	25C19	19NE2	45.62	23O	25C19	23C	14.86
23O	25C19	25N	44.51	23O	25C19	19NE2	58.93
23C	25C19	25N	40.60	23C	25C19	19NE2	45.52
162N	25C19	163N	41.46	162N	25C19	162CE1	69.54
162N	25C19	162CB	28.25	25N	25C19	19NE2	36.78
25N	25C19	163N	74.96	25N	25C19	162CE1	67.79
19NE2	25C19	163N	96.25	19NE2	25C19	162CE1	59.92
163N	25C19	162CE1	51.59	163N	25C19	162CB	39.57
162CE1	25C19	162CB	42.53	161O	25C20	25SG	71.78
161O	25C20	161C	1.07	25SG	25C20	23CA	80.86
25SG	25C20	23O	69.40	25SG	25C20	23C	68.41
25SG	25C20	161C	71.72	23CA	25C20	23O	30.94
23CA	25C20	23C	18.34	23O	25C20	23C	14.77
161O	25C21	161C	6.69	161O	25C22	161C	13.34
161O	25C22	161CA	34.90	161O	25C22	161CB	44.27
161C	25C22	161CA	21.77	161C	25C22	161CB	34.39
161CA	25C22	161CB	20.42	184NE1	25N24	184CZ2	42.68
184NE1	25N24	184CE2	21.38	184NE1	25N24	19OE1	49.07
184NE1	25N24	162ND1	68.83	184NE1	25N24	162CE1	51.55
184NE1	25N24	19CD	58.30	184NE1	25N24	19NE2	75.34
184NE1	25N24	184CD1	9.07	184NE1	25N24	184CH2	51.38
184CZ2	25N24	184CE2	21.94	184CZ2	25N24	19OE1	85.09
184CZ2	25N24	162ND1	64.71	184CZ2	25N24	162CE1	57.67
184CZ2	25N24	19CD	98.31	184CZ2	25N24	184CD1	50.33
184CZ2	25N24	184CH2	9.57	184CE2	25N24	19OE1	68.35
184CE2	25N24	162ND1	68.77	184CE2	25N24	162CE1	55.33
184CE2	25N24	19CD	79.25	184CE2	25N24	19NE2	96.20
184CE2	25N24	184CD1	28.46	184CE2	25N24	184CH2	30.12
19OE1	25N24	162ND1	58.04	19OE1	25N24	162CE1	44.62
19OE1	25N24	19CD	16.03	19OE1	25N24	19NE2	29.68
19OE1	25N24	184CD1	47.21	19OE1	25N24	184CH2	94.65
162ND1	25N24	162CE1	18.14	162ND1	25N24	19CD	72.35
162ND1	25N24	19NE2	76.87	162ND1	25N24	184CD1	75.84
162ND1	25N24	184CH2	69.90	162CE1	25N24	19CD	60.33
162CE1	25N24	19NE2	69.25	162CE1	25N24	184CD1	58.03
162CE1	25N24	184CH2	65.20	19CD	25N24	19NE2	17.04
19CD	25N24	184CD1	53.84	19NE2	25N24	184CD1	70.73
184CD1	25N24	184CH2	58.50	25SG	25C25	25CB	32.75
25SG	25C25	25N	68.12	25SG	25C25	25CA	46.11

TABLE XI

25SG	25C25	19NE2	91.26	25SG	25C25	162ND1	50.45
25SG	25C25	161O	83.98	25SG	25C25	26N	50.26
25SG	25C25	25C	39.24	25SG	25C25	24C	75.91
25SG	25C25	163N	26.06	25SG	25C25	19OE1	68.77
25SG	25C25	162CA	52.77	25SG	25C25	162CE1	48.87
25SG	25C25	24CA	93.64	25SG	25C25	19CD	79.92
25CB	25C25	25N	43.75	25CB	25C25	25CA	22.80
25CB	25C25	23C	96.85	25CB	25C25	19NE2	58.71
25CB	25C25	162ND1	52.80	25CB	25C25	24N	79.85
25CB	25C25	26N	49.57	25CB	25C25	25C	32.45
25CB	25C25	24C	53.95	25CB	25C25	163N	56.86
25CB	25C25	19OE1	39.72	25CB	25C25	162CA	76.70
25CB	25C25	162CE1	41.55	25CB	25C25	24CA	71.02
25CB	25C25	19CD	48.30	25N	25C25	23O	61.20
25N	25C25	25CA	22.53	25N	25C25	23C	54.87
25N	25C25	23CA	71.33	25N	25C25	19NE2	46.58
25N	25C25	162ND1	94.33	25N	25C25	24N	38.82
25N	25C25	26N	37.62	25N	25C25	25C	32.96
25N	25C25	24C	10.58	25N	25C25	163N	94.01
25N	25C25	19OE1	53.89	25N	25C25	162CE1	80.69
25N	25C25	24CA	27.34	25N	25C25	19CD	48.28
23O	25C25	25CA	82.78	23O	25C25	23C	18.78
23O	25C25	23CA	35.84	23O	25C25	19NE2	73.70
23O	25C25	24N	31.06	23O	25C25	26N	72.39
23O	25C25	25C	83.36	23O	25C25	24C	51.02
23O	25C25	19OE1	99.77	23O	25C25	24CA	34.14
23O	25C25	19CD	86.19	25CA	25C25	23C	77.38
25CA	25C25	23CA	92.63	25CA	25C25	19NE2	55.22
25CA	25C25	162ND1	75.50	25CA	25C25	24N	61.07
25CA	25C25	26N	33.30	25CA	25C25	25C	18.88
25CA	25C25	24C	31.91	25CA	25C25	163N	72.17
25CA	25C25	19OE1	48.70	25CA	25C25	162CA	96.87
25CA	25C25	162CE1	63.50	25CA	25C25	24CA	49.61
25CA	25C25	19CD	50.26	23C	25C25	23CA	22.22
23C	25C25	19NE2	55.76	23C	25C25	24N	17.04
23C	25C25	26N	77.83	23C	25C25	25C	83.98
23C	25C25	24C	46.58	23C	25C25	19OE1	82.85
23C	25C25	24CA	28.93	23C	25C25	19CD	68.78
23CA	25C25	19NE2	53.36	23CA	25C25	24N	33.27
23CA	25C25	26N	99.45	23CA	25C25	24C	65.16
23CA	25C25	19OE1	80.77	23CA	25C25	24CA	48.92
23CA	25C25	19CD	66.76	19NE2	25C25	162ND1	78.91
19NE2	25C25	24N	43.72	19NE2	25C25	26N	83.54
19NE2	25C25	25C	73.61	19NE2	25C25	24C	50.86

TABLE XI

19NE2	25C25	19OE1	27.88	19NE2	25C25	162CE1	65.60
19NE2	25C25	24CA	51.46	19NE2	25C25	19CD	13.57
162ND1	25C25	1610	66.11	162ND1	25C25	26N	97.49
162ND1	25C25	25C	81.90	162ND1	25C25	163N	47.00
162ND1	25C25	19OE1	52.01	162ND1	25C25	162CA	38.64
162ND1	25C25	162CE1	14.60	162ND1	25C25	19CD	65.91
1610	25C25	163N	58.15	1610	25C25	162CA	33.71
1610	25C25	162CE1	80.71	24N	25C25	26N	67.35
24N	25C25	25C	70.00	24N	25C25	24C	31.89
24N	25C25	19OE1	68.76	24N	25C25	24CA	16.51
24N	25C25	19CD	55.45	26N	25C25	25C	17.11
26N	25C25	24C	37.71	26N	25C25	163N	70.13
26N	25C25	19OE1	81.99	26N	25C25	162CA	99.71
26N	25C25	162CE1	89.75	26N	25C25	24CA	50.94
26N	25C25	19CD	82.06	25C	25C25	24C	38.11
25C	25C25	163N	63.33	25C	25C25	19OE1	66.63
25C	25C25	162CA	91.85	25C	25C25	162CE1	73.03
25C	25C25	24CA	55.12	25C	25C25	19CD	69.13
24C	25C25	19OE1	62.72	24C	25C25	162CE1	91.22
24C	25C25	24CA	17.90	24C	25C25	19CD	55.23
163N	25C25	19OE1	86.02	163N	25C25	162CA	29.58
163N	25C25	162CE1	53.83	163N	25C25	19CD	99.46
19OE1	25C25	162CA	90.22	19OE1	25C25	162CE1	38.06
19OE1	25C25	24CA	71.30	19OE1	25C25	19CD	14.33
162CA	25C25	162CE1	52.16	162CE1	25C25	19CD	52.25
24CA	25C25	19CD	60.28	25SG	25026	25N	75.08
25SG	25026	25CB	37.30	25SG	25026	25CA	54.02
25SG	25026	24C	86.45	25SG	25026	19CD	97.95
25SG	25026	19OE1	82.42	25SG	25026	25C	45.95
25SG	25026	26N	51.16	25SG	25026	162ND1	46.91
25SG	25026	162CE1	52.51	25N	25026	23C	71.27
25N	25026	25CB	49.91	25N	25026	23CA	95.71
25N	25026	19NE2	63.43	25N	25026	23O	74.28
25N	25026	24N	51.65	25N	25026	25CA	24.00
25N	25026	24C	13.92	25N	25026	19CD	63.32
25N	25026	19OE1	66.78	25N	25026	24CA	35.47
25N	25026	23N	92.49	25N	25026	22O	75.23
25N	25026	25C	29.57	25N	25026	26N	34.00
25N	25026	162ND1	97.43	25N	25026	22C	83.38
25N	25026	162CE1	86.18	23C	25026	23CA	29.24
23C	25026	19NE2	77.74	23C	25026	23O	22.63
23C	25026	24N	23.28	23C	25026	25CA	95.23
23C	25026	24C	57.44	23C	25026	19CD	92.50
23C	25026	24CA	35.81	23C	25026	23N	31.40